FEW-SHOT DOMAIN ADAPTATION BY CAUSAL MECHANISM TRANSFER

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ABSTRACT

We study few-shot supervised domain adaptation (DA) for regression problems, where only a few labeled target domain data and many labeled source domain data are available. Many of the current DA methods base their transfer assumptions on either parametrized distribution shift or apparent distribution similarities, e.g., identical conditionals or small distributional discrepancies. However, these assumptions may preclude the possibility of adaptation from intricately shifted and apparently very different distributions. To overcome this problem, we propose mechanism transfer, a meta-distributional scenario in which a data generating mechanism is invariant among domains. This transfer assumption can accommodate nonparametric shifts resulting in apparently different distributions while providing a solid statistical basis for DA. We take the structural equations in causal modeling as an example and propose a novel DA method, which is shown to be useful both theoretically and experimentally. Our method can be seen as the first attempt to fully leverage the structural causal models for DA.

1 Introduction

Learning from a limited amount of data is a long-standing yet actively studied problem of machine learning. Domain adaptation (DA) [Ben-David et al., 2010] tackles this problem by leveraging auxiliary data sampled from related but different domains. In particular, we consider few-shot supervised DA for regression problems, where only a few labeled target domain data and many labeled source domain data are available.

A key component of DA methods is the transfer assumption (TA) to relate the source and the target distributions. Many of the previously explored TAs have relied on certain direct distributional similarities, e.g., identical conditionals (Shimodaira, 2000) or small distributional discrepancies (Ben-David et al., 2007). However, these TAs may preclude the possibility of adaptation from apparently very different distributions. Many others assume parametric forms of the distribution shift (Zhang et al., 2013) or the distribution family (Storkey and Sugiyama, 2007) which can highly limit the considered set of distributions. (we further review related work in Section 5.1).

To alleviate the intrinsic limitation of previous TAs due to relying on apparent distribution similarities or parametric assumptions, we focus on a meta-distributional scenario where there exists a common generative mechanism behind the data distributions (Figures [1,2]). Such a common mechanism may be more conceivable in applications involving structured table data such as medical records (Yadav et al., 2018). For example, in medical record analysis for disease risk prediction, it can be reasonable to assume that there is a pathological mechanism that is common across regions or generations, but the data distributions may vary due to the difference in cultures or lifestyles. Such a hidden structure (pathological mechanism, in this case), once estimated, may provide portable knowledge to enable DA, allowing one to obtain accurate predictors for under-investigated regions or new generations.

Concretely, our assumption relies on the generative model of nonlinear independent component analysis (nonlinear ICA; Figure [1]), where the observed labeled data are generated by first sampling latent independent components (ICs) $S$ and later transforming them by a nonlinear invertible mixing function denoted by $f$ (Hyvärinen et al., 2019). Under this generative model, our TA is that $f$ representing the mechanism is identical across domains (Figure [2]). This TA
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Our key contributions can be summarized in three points as follows.

1. We formulate the flexible yet intuitively accessible TA of shared generative mechanism and develop a few-shot regression DA method (Section 3). The idea is as follows. First, from the source domain data, we estimate the mixing function $f$ by nonlinear ICA (Hyvärinen et al., 2019) because $f$ is the only assumed relation of the domains. Then, to transfer the knowledge, we perform data augmentation using the estimated $f$ on the target domain data using the independence of the IC distributions. In the end, the augmented data is used to fit a target predictor (Figure 3).

2. We theoretically justify the augmentation procedure by invoking the theory of generalized U-statistics (Lee, 1990). The theory shows that the proposed data augmentation procedure yields the uniformly minimum variance unbiased risk estimator in an ideal case. We also provide an excess risk bound (Mohri et al., 2012) to cover a more realistic case (Section 4).

3. We experimentally demonstrate the effectiveness of the proposed algorithm (Section 6). The real-world data we use is taken from the field of econometrics, for which structural equation models have been applied in previous studies (Greene, 2012).

A salient example of the generative model we consider is the structural equations of causal modeling (Section 2). In this context, our method can be seen as the first attempt to fully leverage the structural causal models for DA (Section 5.2).

2 Problem Setup

In this section, we describe the problem setup and the notation. To summarize, our problem setup is homogeneous, multi-source, and few-shot supervised domain adapting regression. That is, respectively, all data distributions are defined on the same data space, there are multiple source domains, and a limited number of labeled data is available from the target distribution (and we do not assume the availability of unlabeled data). In this paper, we use the terms domain and distribution interchangeably.

Notation. Let us denote the set of real (resp. natural) numbers by $\mathbb{R}$ (resp. $\mathbb{N}$). For $N \in \mathbb{N}$, we define $[N] := \{1, 2, \ldots, N\}$. Throughout the paper, we fix $D(\in \mathbb{N}) > 1$ and suppose that the input space $\mathcal{X}$ is a subset of $\mathbb{R}^{D-1}$ and the label space $\mathcal{Y}$ is a subset of $\mathbb{R}$. As a result, the overall data space $\mathcal{Z} := \mathcal{X} \times \mathcal{Y}$ is a subset of $\mathbb{R}^D$. We generally denote a labeled data point by $Z = (X, Y)$. We denote by $\mathcal{Q}$ the set of independent distributions on $\mathbb{R}^D$ with
We denote $g$ SEMs (Pearl, 2009) under adequate assumptions such as invertibility. SEMs are used to describe the data Markovian whose relations to with identical mixing functions (Figure 2). To be precise, we assume that there exists a set of IC distributions $(GCL; Hyvärinen et al., 2019)$. GCL uses auxiliary information for training a certain binary classification function, $f$. The first step estimates the common transformation $GCL$ is logistic regression to classify of $f$ equipped with a parametrized feature extractor $\hat{f}$ target domain data to transfer the knowledge (Figure 3). In this section, we detail the proposed method, mechanism transfer (Algorithm 1). The method first estimates the common generative mechanism $f$ to solve an easier estimation problem compared to causal discovery. Reduced-form equation can be derived given the structural-form equations by recursive imputation, we are only required assumption of this paper translates into the invariance of the structural equations among domains. Note that we do not their successors (Kano and Shimizu, 2003; Shimizu et al., 2006; Monti et al., 2019). In the case of SEMs, the key generating mechanism involving the causality of random variables (Pearl, 2009). This interpretation of SEMs as Eq.(1) (SEMs; Pearl, 2009; Peters et al., 2017), more precisely, the reduced form (Reiss and Wolak, 2007) of Example: Structural equation models  A salient example of generative models expressed as Eq. (1) is structural equation models (SEMs; Pearl 2009 Peters et al. 2017), more precisely, the reduced form (Reiss and Wolak 2007) of Markovian SEMs (Pearl 2009) under adequate assumptions such as invertibility. SEMs are used to describe the data generating mechanism involving the causality of random variables (Pearl 2009). This interpretation of SEMs as Eq.(1) has been exploited in methods of causal structure discovery such as the linear non-Gaussian additive-noise models and their successors (Kano and Shimizu 2003; Shimizu et al. 2006; Monti et al. 2019). In the case of SEMs, the key assumption of this paper translates into the invariance of the structural equations among domains. Note that we do not require the estimation of the exact structural equations, but only the reduced form needs to be estimated. Since the reduced-form equation can be derived given the structural-form equations by recursive imputation, we are only required to solve an easier estimation problem compared to causal discovery.

### 3 Proposed Method: Mechanism Transfer

In this section, we detail the proposed method, mechanism transfer (Algorithm 1). The method first estimates the common generative mechanism $f$ from the source domain data and then uses it to perform data augmentation of the target domain data to transfer the knowledge (Figure 3).

#### 3.1 Step 1: Estimate $f$ using the source domain data

The first step estimates the common transformation $f$ by nonlinear ICA, namely by generalized contrastive learning (GCL; Hyvärinen et al. 2019). GCL uses auxiliary information for training a certain binary classification function, $r_{f, \psi}$, equipped with a parametrized feature extractor $f : \mathbb{R}^D \rightarrow \mathbb{R}^D$. The trained feature extractor $\hat{f}$ is used as an estimator of $f$. The auxiliary information we use in our problem setup is the domain indices $[K]$. The classification function to be trained in GCL is $r_{f, \phi}(z, u) := \sum_{d=1}^D \psi_d(f^{-1}(z), u)$ consisting of $(f, \{\psi_d\}_{d=1}^D)$, and the classification task of GCL is logistic regression to classify $(Z_{k, i}^{\text{Src}}, k)$ as positive and $(Z_{k', i}^{\text{Src}}, k' \neq k)$ as negative. This yields the following
Algorithm 1 Proposed method: mechanism transfer

**Input:** Source domain data sets \( \{D_k\}_{k \in [K]} \), target domain data set \( D_{\text{Tar}} \), nonlinear ICA algorithm \( \text{ICA} \), and a learning algorithm \( \mathcal{A}_G \) to fit the hypothesis class \( \mathcal{G} \) of predictors.

// Step 1. Estimate the shared transformation.
\[
\hat{f} \leftarrow \text{ICA}(D_1, \ldots, D_K)
\]

// Step 2. Extract and shuffle target independent components
\[
\hat{s}_i \leftarrow \hat{f}^{-1}(Z_i), \quad (i = 1, \ldots, n_{\text{Tar}})
\]
\[
\{\hat{s}_i\}_{i \in [n_{\text{Tar}}]} \leftarrow \text{AllCombinations}\{\hat{s}_i\}_{i=1}^{n_{\text{Tar}}}
\]

// Step 3. Synthesize target data and fit the predictor.
\[
\hat{g} \leftarrow \mathcal{A}_G\{\hat{s}_i\}_i
\]

**Output:** \( \hat{g} \): the predictor in the target domain.

Domain-contrastive learning criterion to estimate \( \hat{f} \):
\[
\arg\min_{f \in \mathcal{F}} \sum_{k=1}^K \sum_{i=1}^{n_k} \phi\left( r_{f,\psi}(Z_{i,k}^{\text{Src}}, k) \right) + \mathbb{E}_{k' \neq k} r_{f,\overline{\psi}}(Z_{i,k}^{\text{Src}}, k')
\]
where \( \mathcal{F} \) and \( \Psi \) are sets of parametrized functions, \( \mathbb{E}_{k' \neq k} \) denotes the expectation with respect to \( k' \sim U([K] \setminus \{k\}) \) (\( U \) denotes the uniform distribution), and \( \phi \) is the logistic loss \( \phi(m) := \log(1 + \exp(-m)) \). We use the solution \( \hat{f} \) as an estimator of \( f \). In experiments, \( \mathcal{F} \) is implemented by invertible neural networks \( \text{Kingma and Dhariwal} \) \( 2018 \), \( \Psi \) by multi-layer perceptron, and \( \mathbb{E}_{k' \neq k} \) is replaced by a random sampling renewed for every mini-batch.

3.2 Step 2: Extract and inflate the target ICs using \( \hat{f} \)

The second step extracts and inflates the target domain ICs using the estimated \( \hat{f} \). We first extract the ICs of the target domain data by applying the inverse of \( \hat{f} \) as
\[
\hat{s}_i = \hat{f}^{-1}(Z_i).
\]
After the extraction, we inflate the set of IC values by taking all dimension-wise combinations of the estimated IC:
\[
\bar{s}_i = (\hat{s}_{i,1}, \ldots, \hat{s}_{i,D}), \quad i = (i_1, \ldots, i_D) \in [n_{\text{Tar}}]^D,
\]
to obtain new plausible IC values \( \bar{s}_i \). The intuitive motivation of this procedure stems from the independence of the IC distributions. Theoretical justifications are provided in Section 4. In our implementation, we use invertible neural networks \( \text{Kingma and Dhariwal} \) \( 2018 \) to model the function \( \hat{f} \) to enable the computation of the inverse \( \hat{f}^{-1} \).

3.3 Step 3: Synthesize target data from the inflated ICs

The third step estimates the target risk \( \hat{R} \) by the empirical distribution of the augmented data:
\[
\hat{R}(g) := \frac{1}{n_{\text{Tar}}} \sum_{i \in [n_{\text{Tar}}]} \ell(g, \hat{f}(\hat{s}_i)), \quad (2)
\]
and performs empirical risk minimization. In experiments, we use a regularization term \( \Omega(\cdot) \) to control the complexity of \( \mathcal{G} \) and select
\[
\hat{g} \in \arg\min_{g \in \mathcal{G}} \{ \hat{R}(g) + \Omega(g) \}.
\]
The generated hypothesis \( \hat{g} \) is then used to make predictions in the target domain. In our experiments, we use \( \Omega(g) = \lambda \|g\|^2 \), where \( \lambda > 0 \) and the norm is that of the reproducing kernel Hilbert space (RKHS) which we take the subset \( \mathcal{G} \) from. Note that we may well reduce the computing time by taking only a subset of combinations in Eq. (2).
4 Theoretical Insights

In this section, we state two theorems to investigate the statistical properties of the method proposed in Section 3 and provide plausibility beyond the intuition that we take advantage of the independence of the IC distributions.

4.1 Minimum variance property: Idealized case

The first theorem provides an insight into the statistical advantage of the proposed method: in the ideal case, the method attains the minimum variance among all possible unbiased risk estimators.

**Theorem 1** (Minimum variance property of $\hat{R}$). Assume that $\hat{f} = f$. Then, for each $g \in \mathcal{G}$, the proposed risk estimator $\hat{R}(g)$ is the uniformly minimum variance unbiased estimator of $R(g)$, i.e., for any unbiased estimator $\tilde{R}(g)$ of $R(g)$,

$$\forall q \in Q, \quad \text{Var}(\tilde{R}(g)) \leq \text{Var}(\hat{R}(g))$$

as well as $\mathbb{E}_{\mathcal{G}^{n}} \hat{R}(g) = R(g)$ holds.

The proof of Theorem 1 is immediate once we rewrite $R(g)$ as a $D$-variate regular statistical functional and $\hat{R}(g)$ as its corresponding generalized U-statistic [Lee, 1990]. Details can be found in Supplementary Material [D] Theorem 1 implies that the proposed risk estimator can have superior statistical efficiency in terms of the variance over the ordinary empirical risk.

4.2 Excess risk bound: More realistic case

In real situations, one has to estimate $f$. The following theorem characterizes the statistical gain and loss arising from the estimation error $f - \hat{f}$. The intuition is that the increased number of points suppresses the possibility of overfitting because the hypothesis has to fit the majority of the inflated data, but the estimator $\hat{f}$ has to be accurate so that fitting to the inflated data is meaningful. Note that the theorem is agnostic to how $\hat{f}$ is obtained, hence it applies to more general problem setup as long as $\hat{f}$ can be estimated.

**Theorem 2** (Excess risk bound). Let $\tilde{g}$ be the hypothesis generated by Eq. (2). Under appropriate assumptions (see Theorem 3 [in Supplementary Material]), for arbitrary $\delta, \delta' \in (0, 1)$, we have with probability at least $1 - (\delta + \delta')$,

$$R(\tilde{g}) - R(g^*) \leq C \sum_{j=1}^{D} \left| f_{j} - \hat{f}_{j} \right|_{W^{1,1}} + 4DR(\tilde{g}) + 2DB_{\ell} \sqrt{\frac{\log 2/\delta}{2n}} + \kappa_1(\delta', n) + DB_{\ell}B_{q}\kappa_2(f - \hat{f}).$$

Here, $\left| \cdot \right|_{W^{1,1}}$ is the $(1, 1)$-Sobolev norm, and we define the effective Rademacher complexity $R(\tilde{g})$ by

$$R(\tilde{g}) := \frac{1}{n} \mathbb{E}_{\tilde{g}} \mathbb{E}_{\sigma} \left[ \sup_{\tilde{g} \in \mathcal{G}} \left| \sum_{i=1}^{n} \sigma_{i} \mathbb{E}_{\tilde{S}_{i}^{1}, \ldots, \tilde{S}_{i}^{D}} \left[ \hat{\ell}(\tilde{s}_{i}, \tilde{S}', \ldots, \tilde{S}') \right] \right| \right],$$

where $\{\sigma_{i}\}_{i=1}^{n}$ are independent sign variables, $\mathbb{E}_{\tilde{g}}$ is the expectation with respect to $\left\{ \tilde{s}_{i} \right\}_{i=1}^{n}$, the dummy variables $\tilde{S}', \ldots, \tilde{S}'_{D}$ are i.i.d. copies of $\tilde{s}_{i}$, and $\hat{\ell}$ is defined by using the degree-$D$ symmetric group $\mathcal{G}_{D}$ as

$$\hat{\ell}(\tilde{s}_{1}, \ldots, \tilde{s}_{D}) := \frac{1}{D!} \sum_{\pi \in \mathcal{G}_{D}} \ell(g, \tilde{f}(\tilde{s}_{1}^{(1)}, \ldots, \tilde{s}_{D}^{(D)}),$$

and $\kappa_1(\delta', n)$ and $\kappa_2(f - \hat{f})$ are higher order terms. The constants $B_{q}$ and $B_{\ell}$ depend only on $q$ and $\ell$, respectively, while $C_{\delta}$ depends only on $f, q, \ell,$ and $D$.

Details of the statement and the proof can be found in Supplementary Material [D]. The Sobolev norm [Adams and Fournier, 2003] emerges from the evaluation of the difference between the estimated IC distribution and the ground-truth IC distribution. In Theorem 2, the utility of the proposed method appears in the effective complexity measure. The complexity is defined by a set of functions which are marginalized over all but one argument, resulting in mitigated dependence on the input dimensionality from exponential to linear (Supplementary Material [C] Remark 3).

5 Related Work and Discussion

In this section, we review some existing TAs for DA to clarify the relative position of the paper. We also clarify the relation to the literature of causality-related transfer learning.
Table 1: Comparison of TAs for DA (Parametric: parametric distribution family or distribution shift, Invariant dist.: invariant distribution components such as conditionals, marginals, or copulas. Disc. / IPM: small discrepancy or integral probability metric, Param-transfer: existence of transferable parameter, Mechanism: invariant mechanism). AD: adaptation among Apparently Different distributions is accommodated. NP: Non-Parametrically flexible. BCI: Brain computer interface. The numbers indicate the paragraphs of Section 5.1.

| TA                  | AD | NP | Suited app. example |
|---------------------|----|----|---------------------|
| (1) Parametric      | ✓  | -  | Remote sensing      |
| (2) Invariant dist. |    | ✓  | BCI                 |
| (3) Disc. / IPM     | -  | ✓  | Computer vision     |
| (4) Param-transfer  | ✓  | ✓  | Computer vision     |
| (Ours) Mechanism    | ✓  | ✓  | Medical records     |

5.1 Existing transfer assumptions

Here, we review some of the existing work and TAs. See Table 1 for a summary.

(1) **Parametric assumptions.** Some TAs assume parametric distribution families, e.g., Gaussian mixture model in covariate shift (Storkey and Sugiyama, 2007). Some others assume parametric distribution shift, i.e., parametric representations of the target distribution given the source distributions. Examples include location-scale transform of class conditionals (Zhang et al., 2013; Gong et al., 2016), linearly dependent class conditionals (Zhang et al., 2015), and low-dimensional representation of the class conditionals after kernel embedding (Stojanov et al., 2019). In some applications, e.g., remote sensing, some parametric assumptions have proven useful (Zhang et al., 2013).

(2) **Invariant conditionals and marginals.** Some methods assume invariance of certain conditionals or marginals (Quiñonero-Candela et al., 2009), e.g., \( p(Y|X) \) in the covariate shift scenario (Shimodaira, 2000), \( p(Y|T(X)) \) for an appropriate feature transformation \( T \) in transfer component analysis (Pan et al., 2011), \( p(Y|T(X)) \) for a feature selection \( T \) in Rojas-Carulla et al. (2018), \( p(X|Y) \) in the target shift (TarS) scenario (Zhang et al., 2013; Nguyen et al., 2016), and few components of regular-vine copulas and marginals in Lopez-paz et al. (2012). For example, the covariate shift scenario has been shown to fit well to brain computer interface data (Sugiyama et al., 2007).

(3) **Small discrepancy or integral probability metric.** Another line of work relies on certain distributional similarities, e.g., integral probability metric (Courty et al., 2017) or hypothesis-class dependent discrepancies (Ben-David et al., 2007; Blitzer et al., 2008; Ben-David et al., 2010; Kuroki et al., 2019; Zhang et al., 2019; Cortes et al., 2019). These methods assume the existence of the ideal joint hypothesis (Ben-David et al., 2010), corresponding to a relaxation of the covariate shift assumption. These TAs are suited for unsupervised or semi-supervised DA in computer vision applications (Courty et al., 2017).

(4) **Transferable parameter.** Some others consider parameter transfer (Kumaga, 2016), where the TA is the existence of a parameterized feature extractor that performs well in the target domain for linear-in-parameter hypotheses and its learnability from the source domain data. For example, such a TA has been known to be useful in natural language processing or image recognition (Lee et al., 2009; Kumaga, 2016).

5.2 Causality for transfer learning

Our method can be seen as the first attempt to fully leverage structural causal models for DA. Most of the causality-inspired DA methods express their assumptions in the level of graphical causal models (GCMs), which only has much coarser information than structural causal models (SCMs) (Peters et al., 2017, Table 1.1) exploited in this paper. Compared to previous work, our method takes one step further to assume and exploit the invariance of SCMs. Specifically, many studies assume the GCM \( X \leftarrow Y \) (the anticausal scenario) following the seminal meta-analysis of Schölkopf et al. (2012) and use it to motivate their parametric distribution shift assumptions or the parameter estimation procedure (Zhang et al., 2013; 2015; Gong et al., 2016; 2018). Although such assumptions on the GCM have the virtue of being more robust to misspecification, they tend to require parametric assumptions to obtain theoretical justifications. On the other hand, our assumption enjoys a theoretical guarantee without relying on parametric assumptions.
5.3 Plausibility of the assumption

The invariance of causal mechanisms has been exploited in recent work of causal discovery such as Xu et al. (2014) and Monti et al. (2019), or under the name of the multi-environment setting in Ghassami et al. (2017). The SEMs are normally assumed to remain invariant unless explicitly intervened in Hünernund and Bareinboim (2019). As the first algorithm in the approach to fully exploit SCMs for DA, we consider the case where all variables are observable. Although it is often assumed in a causal inference problem that there are some unobserved confounding variables, we leave further extension to such a case for future work.

The relation between $X$ and $Y$ can drastically change while $f$ is invariant. For example, even in a simple additive noise model $(X, Y) = f(S_1, S_2) = (S_1, S_1 + S_2)$, the conditional $p(Y|X)$ can shift drastically if the distribution of the independent noise $S_2$ changes in a complex manner, e.g., becoming multimodal from unimodal.

6 Experiment

In this section, we provide proof-of-concept experiments to demonstrate the effectiveness of the proposed approach. Note that the primary purpose of the experiments is to confirm whether the proposed method can properly perform DA in real-world data, and it is not to determine which DA method and TA are the most suited for the specific dataset.

6.1 Implementation details of the proposed method

Estimation of $f$ (Step 1). We model $\hat{f}$ by an 8-layer Glow neural network (Supplementary Material B.2). We model $\psi_d$ by a 1-hidden-layer neural network with a varied number of hidden units, $K$ output units, and the rectified linear unit activation $\psi_d(x)$ (LeCun et al., 2015). We use its $k$-th output ($k \in \{K\}$) as the value for $\psi_d(\cdot, k)$. For training, we use the Adam optimizer (Kingma and Ba, 2017) with fixed parameters $(\beta_1, \beta_2, \epsilon) = (0.9, 0.999, 10^{-8})$, fixed initial learning rate $10^{-3}$, and the maximum number of epochs 300. The other fixed hyperparameters of $f$ and its training process are described in Supplementary Material B.

Augmentation of target data (Step 3). For each evaluation step, we take all combinations (with replacement) of the estimated ICs to synthesize target domain data. After we synthesize the data, we filter them by applying a novelty detection technique with respect to the union of source domain data. Namely, we use one-class support vector machine (Schölkopf et al., 2000) with the fixed parameter $\nu = 0.1$ and radial basis function (RBF) kernel $k(x, y) = \exp(-\|x - y\|^2/\gamma)$ with $\gamma = D$. This is because the estimated transform $\hat{f}$ is not expected to be trained well outside the union of the supports of the source distributions.

Predictor hypothesis class $G$. As the predictor model, we use the kernel ridge regression (KRR) with RBF kernel. The bandwidth $\gamma$ is chosen by the median heuristic similarly to Yamada et al. (2011) for simplicity. Note that the choice of the predictor model is for the sake of comparison with the other methods tailored for KRR (Cortes et al., 2019), and that an arbitrary predictor hypothesis class and learning algorithm can be easily combined with the proposed approach.

Hyperparameter selection. We perform grid-search for hyperparameter selection. The number of hidden units for $\psi_d$ is chosen from $\{10, 20\}$ and the coefficient of weight-decay from $10^{(-2, -1)}$. The $\ell^2$ regularization coefficient $\lambda$ of KRR is chosen from $\lambda \in 2^{(-10,...,-1)}$ following Cortes et al. (2019). To perform hyperparameter selection as well as early-stopping, we record the leave-one-out cross-validation (LOOCV) mean-squared error on the target training data every 20 epochs and select its minimizer. The leave-one-out score is computed using the well-known analytic formula instead of training the predictor for each split. Note that we only use the original target domain data and not the synthesized data as the held-out set.

Computation environment All experiments were conducted on an Intel Xeon(R) 2.60 GHz CPU with 132 GB memory. They were implemented in Python using the PyTorch library (Paszke et al., 2019) or the R language (R Core Team, 2018).

6.2 Experiment using real-world data

Dataset. We use the gasoline consumption data (Greene, 2012, p.284, Example 9.5), which is a panel data of gasoline usage in 18 of the OECD countries over 19 years. We consider each country as a domain, and we disregard the time-series structure and consider the data as i.i.d. samples for each country in this proof-of-concept experiment. The dataset contains four variables, all of which are log-transformed: motor gasoline consumption per car (the predicted
variable), per-capita income, motor gasoline price, and the stock of cars per capita (the predictor variables) (Baltagi and Griffin, 1983). For further details of the data, see Supplementary Material B. We used the dataset because there are very few public datasets for domain adapting regression tasks (Cortes and Mohri, 2014) especially for multi-source DA, and also because the dataset has been used in econometric analyses involving SEMs (Baltagi, 2005), conforming to our approach.

**Compared methods.** We compare the following DA methods, all of which apply to regression problems. Unless explicitly specified, the predictor class G is chosen to be KRR with the same hyperparameter candidates as the proposed method (Section 6.1). Further details are described in Supplementary Material B.5.

- **Naive baselines (SrcOnly, TrgOnly, and S&TV):** SrcOnly (resp. TrgOnly) trains a predictor on the source domain data (resp. target training data) without any device. SrcOnly can be effective if the source domains and the target domain have highly similar distributions. The S&TV baseline trains on both source and target domain data, but the LOOCV score is computed only from the target domain data.

- **TrAdaBoost:** Two-stage TrAdaBoost.R2; a boosting method tailored for few-shot regression transfer proposed in Pardoe and Stone (2010). It is an iterative method with early-stopping (Pardoe and Stone, 2010), for which we use the leave-one-out cross-validation score on the target domain data as the criterion. As suggested in Pardoe and Stone (2010), we set the maximum number of outer loop iterations at 30. The base predictor is the decision tree regressor with the maximum depth 6 (Hastie et al., 2009). Note that although TrAdaBoost does not have a clarified transfer assumption, we compare the performance for reference.

- **IW:** Importance weighted KRR using RuLSIF (Yamada et al., 2011). The method directly estimates a relative joint density ratio function $\frac{p_{\text{Src}}(x)}{\alpha p_{\text{Src}}(x) + (1-\alpha)p_{\text{Trg}}(x)}$ for $\alpha \in [0, 1)$, where $p_{\text{Src}}$ is a hypothetical source distribution created by pooling all source domain data. Following Yamada et al. (2011), we experiment on $\alpha \in \{0, 0.5, 0.95\}$ and report the results separately. The regularization coefficient $\lambda$ is selected from $\lambda' \in 2^{\{-10,...,10\}}$ using importance-weighted cross-validation (Sugiyama et al., 2007).

- **GDM:** Generalized discrepancy minimization (Cortes et al., 2019). This method performs instance-weighted training on the source domain data with the weights that minimize the generalized discrepancy (via quadratic programming). We select the hyper-parameters $\lambda$, from $2^{\{-10,...,10\}}$ as suggested by Cortes et al. (2019). The selection criterion is the performance of the trained predictor on the target training labels as the method trains on the source domain data and the target unlabeled data.

- **Copula:** Non-parametric regular-vine copula method (Lopez-paz et al., 2012). This method presumes using a specific joint density estimator called regular-vine (R-vine) copulas. Adaptation is realized in two steps: the first step estimates which components of the constructed R-vine model are different by performing two-sample tests based on maximum mean discrepancy (Lopez-paz et al., 2012), and the second step re-estimates the components in which a change is detected using only the target domain data.

- **LOO (reference score):** Leave-one-out cross-validated error estimate is also calculated for reference. It is the average prediction error of predicting for a single held-out test point when the predictor is trained on the rest of the whole target domain data including those in the test set for the other algorithms.

**Evaluation procedure.** The prediction accuracy was measured by the mean squared error (MSE). For each train-test split, we randomly select one-third (6 points) of the target domain dataset as the training set and use the rest as the test set. All experiments were repeated 10 times with different train-test splits of target domain data.

**Results.** The results are reported in Table 2. We report the MSE scores normalized by that of LOO to facilitate the comparison, similarly to Cortes and Mohri (2014). In many of the target domain choices, the naive baselines (SrcOnly and S&TV) suffer from negative transfer, i.e., higher average MSE than TarOnly (in 12 out of 18 domains). On the other hand, the proposed method successfully performs better than TarOnly or is more resistant to negative transfer than the other compared methods. The performances of GDM, Copula, and IW are often inferior even compared to the baseline performance of SrcAndTarValid. For GDM and IW, this can be attributed to the fact that these methods presume the availability of abundant (unlabeled) target domain data, which is unavailable in the current problem setup. For Copula, the performance inferior to the naive baselines is possibly due to the restriction of the predictor model to its accompanied probability model (Lopez-paz et al., 2012). TrAdaBoost works reasonably well for many but not all domains. For some domains, it suffered from negative transfer similarly to others, possibly because of the very small number of training data points. Note that the transfer assumption of TrAdaBoost has not been stated (Pardoe and Stone, 2010), and it is not understood when the method is reliable.
Table 2: Results of the real-world data experiments for different choices of the target domain. The evaluation score is MSE normalized by that of LOO (the lower the better). All experiments were repeated 10 times with different train-test splits of target domain data, and the average performance is reported with the standard errors in the brackets. The target column indicates abbreviated country names. Bold-face indicates the best score (Prop: proposed method, TrAda: TrAdaBoost), the numbers in the brackets of IW indicate the value of $\alpha$. The proposed method often improves upon the baseline TrgOnly or is relatively more resistant to negative transfer, with notable improvements in DEU, GBR, and USA.

| Target | (LOO) | TrgOnly | Prop | SrcOnly | S&TV | TrAda | GDM | Copula | IW(.0) | IW(.5) | IW(95) |
|--------|-------|---------|------|---------|------|-------|-----|-------|--------|--------|--------|
| AUT    | 5.88  | 3.59    | 5.39 | 9.67    | 9.84 | 8.78  | 3.78 | 31.56 | 27.33  | 39.72  | 39.45  | 39.18  |
| BEL    | 10.70 | 7.94    | 2.19 | 8.19    | 9.48 | 8.10  | 8.10 | 89.10 | 119.86 | 105.15 | 105.28 | 104.30 |
| CAN    | 5.16  | 3.84    | 0.98 | 15.77   | 16.65| 51.94 | 51.90| 510.91| 592.41 | 591.21 | 589.87 |
| DNK    | 3.26  | 3.23    | 0.63 | 30.79   | 29.12| 25.60 | 16.84| 14.46 | 22.28  | 22.11  | 21.72  |
| FRA    | 2.79  | 1.92    | 0.66 | 4.67    | 3.06 | 32.65 | 9.19 | 116.29| 116.54 | 116.64 | 115.29 |
| DEU    | 16.99 | 6.71    | 1.23 | 229.65  | 210.59| 341.03| 73.99| 929.03| 817.50 | 818.13 | 812.60 |
| GRC    | 3.80  | 3.55    | 1.79 | 5.30    | 5.75 | 11.78 | 26.90| 23.05 | 47.07  | 45.50  | 45.72  |
| IRL    | 3.05  | 3.04    | 0.34 | 4.35    | 135.57| 12.34 | 23.40| 3.84  | 26.60  | 6.38   | 6.31   |
| ITA    | 13.00 | 6.71    | 4.15 | 14.05   | 39.27 | 87.34 | 226.95| 343.10| 244.25 | 244.84 | 242.60 |
| JPN    | 10.55 | 12.32   | 4.95 | 8.10    | 8.38 | 18.81 | 95.58 | 71.02 | 135.24 | 134.89 | 134.16 |
| NLD    | 3.75  | 3.87    | 0.79 | 0.99    | 0.99 | 4.95  | 28.35 | 29.53 | 33.28  | 33.23  | 33.14  |
| NOR    | 2.70  | 2.82    | 0.73 | 1.86    | 1.63 | 24.25 | 23.36 | 31.37 | 27.86  | 27.86  | 27.52  |
| ESP    | 5.18  | 6.09    | 1.53 | 5.17    | 4.29 | 14.85 | 33.16 | 152.59| 53.53  | 52.56  | 52.06  |
| SWE    | 6.44  | 5.47    | 2.63 | 2.48    | 2.02 | 2.18  | 15.53 | 270.85| 118.46 | 118.23 | 118.27 |
| CHE    | 3.51  | 2.90    | 0.37 | 43.59   | 7.48 | 38.32 | 8.43  | 29.71 | 9.72   | 9.71   | 9.79   |
| TUR    | 1.65  | 1.06    | 0.47 | 1.22    | 0.91 | 2.19  | 64.26 | 142.84| 159.79 | 157.89 | 157.13 |
| GBR    | 5.95  | 2.66    | 0.57 | 15.92   | 10.05| 7.57  | 50.04 | 68.70 | 70.98  | 70.87  | 69.72  |
| USA    | 4.98  | 1.60    | 0.42 | 21.53   | 12.28| 2.06  | 308.69| 244.90| 462.51 | 464.75 | 465.88 |

#Best - 2 10 2 4 0 0 0 0 0 0 0

7 Conclusion

In this paper, we proposed a novel few-shot supervised DA method for regression problems based on the assumption of shared generative mechanism. Through theoretical and experimental analysis, we demonstrated the effectiveness of the proposed approach. By considering the latent common structure behind the domain distributions, the proposed method successfully induces positive transfer even when a naive usage of the source domain data can suffer from negative transfer. Our future work includes making an experimental comparison with extensively more datasets and methods as well as an extension to the case where the underlying mechanism are not exactly identical but similar.
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Appendices

This is the Supplementary Material for “Few-shot Domain Adaptation by Causal Mechanism Transfer.” Table 3 summarizes the abbreviations and the symbols used in the paper.

A Preliminary: Nonlinear ICA

Here, we use the same notation as the main text. The recently developed nonlinear ICA provides an algorithm to estimate the mixing function $f$. For the case of nonlinear $f$, the impossibility of identification (i.e., consistent estimation) of $f$ in the one-sample i.i.d. case had been established more than two decades ago (Hyvärinen and Pajunen, 1999). However, recently, various conditions have been proposed under which $f$ can be identified with the help of auxiliary information (Hyvärinen and Morioka, 2016, 2017; Hyvärinen et al., 2019; Khemakhem et al., 2019).

The identification condition that is directly relevant to this paper is that of the generalized contrastive learning (GCL) proposed in Hyvärinen et al. (2019). Hyvärinen et al. (2019) assumes that an auxiliary variable $u_i$ from some measurable set $U$ is obtained for each data point as $\{(z_i, u_i)\}_{i=1}^n$ and that the ICs $S = (S^{(1)}, \ldots, S^{(D)})$ are conditionally independent given $u$:

$$q(s|u) = \sum_{d=1}^{D} q^{(d)}(s^{(d)}|u).$$

Under such conditions, GCL estimates $f$ by training a classification function

$$r_{f, \phi}(z, u) = \sum_{d=1}^{D} \psi_d(f^{-1}(z), u) \quad (4)$$

parametrized by $\hat{f}$ and $\{\psi_d\}_{d=1}^{D}$ with the logistic loss for classifying $(z, u)$ vs. $(z, \tilde{u})$,

where $\tilde{u} \in U \setminus \{u\}$. The key condition for the identification of $f$ is the following.

Assumption 1 (Assumption of variability; Hyvärinen et al. [2019], Theorem 1). For any $z$, there exist $2D + 1$ distinct points in $U$, denoted by $\{u_j\}_{j=0}^{2D}$, such that the set of $(2D)$-dimensional vectors $\{w(z|u_j) - w(z|u_0)\}_{j=1}^{2D}$ are linearly independent, where

$$w(z|u) := \left(\frac{\partial q^{(1)}(z_1|u)}{\partial z_1}, \ldots, \frac{\partial q^{(D)}(z_D|u)}{\partial z_D}, \frac{\partial^2 q^{(1)}(z_1|u)}{\partial z_1^2}, \ldots, \frac{\partial^2 q^{(D)}(z_D|u)}{\partial z_D^2}\right).$$

Under Assumption 1 and some regularity conditions, Theorem 1 of Hyvärinen et al. (2019) states that the transformation $\hat{f}$ in Eq. (4) trained by GCL is a consistent estimator of $f$ up to additional dimension-wise invertible transformations. Note that the assumption is intrinsically difficult to confirm based on data due to the unsupervised nature of the problem setting. In this paper, we use the source domain index as the auxiliary variable and employ GCL for domain adaptation. The present version of Assumption 1 requires that we have at least $2D + 1$ distinct source domains. Although this condition can be restrictive in high-dimensional data, we conjecture that there is a possibility for this assumption to be made less stringent in the future because the identification condition is only known to be a sufficient condition, not a necessary condition. However, pursuing a refinement of the identification condition is out of the scope of this paper. Among the various methods for nonlinear ICA, we chose to use GCL (Hyvärinen et al., 2019) because it can operate under a nonparametric assumption on the IC distributions whereas other nonlinear ICA methods (Hyvärinen and Morioka, 2016, 2017; Khemakhem et al., 2019) may require parametric assumptions.

B Experiment Details

Here, we describe more implementation details of the experiment. We plan to publish the experiment code and the dataset if the manuscript is accepted for publication. A URL to the experiment code will appear here.
Table 3: List of abbreviations and symbols used in the paper.

| Abbreviation / Symbol | Meaning |
|-----------------------|---------|
| DA                    | Domain adaptation |
| TA                    | Transfer assumption |
| SEM                   | Structural equation model |
| GCM                   | Graphical causal model |
| SCM                   | Structural causal model |
| IC                    | Independent component |
| ICA                   | Independent component analysis |
| GCL                   | Generalized contrastive learning |
| i.i.d.                | Independent and identically distributed |
| \([N]\)               | \(\{1, 2, \ldots, N\}\) where \(N \in \mathbb{N}\) |
| \(\|W_{k,p}\|_{W^{k,p}}\) | The \((k, p)\)-Sobolev norm |
| \(X \in \mathbb{R}^{D-1}\) | The predictor random vector |
| \(Y \in \mathbb{R}\) | The predicted random variable |
| \(Z = (X, Y) \in \mathbb{R}^D\) | The joint random variable |
| \(S \in \mathbb{R}^D\) | The independent component vector |
| \(X \subset \mathbb{R}^{D-1}\) | The space of \(X\) |
| \(Y \subset \mathbb{R}\) | The space of \(Y\) |
| \(Z \subset \mathbb{R}^D\) | The space of \(Z = (X, Y)\) |
| \(\mathcal{G} \subset \{g : \mathbb{R}^{D-1} \to \mathbb{R}\}\) | Predictor hypothesis class |
| \(\ell : \mathcal{G} \times Z \to [0, B_\ell]\) | Loss function |
| \(R(g)\) | Target domain risk \(E_{p_{\text{Tar}}} \ell(g, Z)\) |
| \(g^* \in \mathcal{G}\) | Minimizer of target domain risk |
| \(Q\) | The set of independent distributions |
| \(f\) | Ground truth mixing function |
| \(p_{\text{Tar}}\) | The target joint distribution |
| \(p_k\) | The joint distribution of source domain \(k\) |
| \(q_{\text{Tar}} \in Q\) | The target independent component (IC) distribution |
| \(q_k \in Q\) | The IC distribution of source domain \(k\) |
| \(D\) | The dimension of \(Z\) |
| \(K\) | The number of source domains |
| \(n_{\text{Tar}}\) | The size of the target labeled sample |
| \(n_k\) | The size of the labeled sample from source domain \(k\) |
| \(\mathcal{D}_{\text{Tar}} = \{Z_i\}_{i=1}^{n_{\text{Tar}}}\) | Target labeled data set |
| \(\mathcal{D}_k = \{Z_{k,i}\}_{i=1}^{n_k}\) | Source labeled data set of source domain \(k\) |
| \(\hat{R}(g)\) | The ordinary empirical risk estimator |
| \(\hat{R}(g)\) | The proposed risk estimator (Eq. (2)) |
| \(\hat{f}\) | The estimator of \(f\) |
| \(\{\psi_d\}_{d=1}^D\) | The penultimate layer functions composed with \(f\) during GCL |

B.1 Dataset details

Gasoline consumption data. The data was downloaded from [http://bcs.wiley.com/he-bcs/Books?action=resource&bcsId=4338&itemId=1118672321&resourceId=13452](http://bcs.wiley.com/he-bcs/Books?action=resource&bcsId=4338&itemId=1118672321&resourceId=13452)

B.2 Model details: Invertible neural networks

Here, we describe the details of the Glow architecture ([Kingma and Dhariwal, 2018](http://bcs.wiley.com/he-bcs/Books?action=resource&bcsId=4338&itemId=1118672321&resourceId=13452)) used in our experiments. Glow consists of three types of layers which are invertible by design, namely affine coupling layers, \(1 \times 1\) convolution layers, and actnorm layers. In our implementation, we do not include actnorm layers, and each layer of our Glow architecture consist of a \(1 \times 1\) convolution layer followed by an affine coupling layer.

**Affine coupling layers.** The coefficients \(s\) and \(t\) for affine coupling layers in the notation of [Kingma and Dhariwal, 2018](http://bcs.wiley.com/he-bcs/Books?action=resource&bcsId=4338&itemId=1118672321&resourceId=13452) are parametrized by two one-hidden-layer neural networks whose number of hidden units is the same and the first layer parameter is shared. The activation functions of the first layer, the second layer of \(s\), and the second layer of
We initialize the parameters for each layer of \( \psi \) we omit the domain identifiers from the distributions and the sample size, such as \( \text{Tar} \). To make the proof self-contained, we first recall some general and problem-specific notation. In the notation here, \( 1 \times D_a \) denotes a finite set \( A \) any \( N \) elements. For a vector \( x \) and \( Dhariwal, 2018 \), we define its \( \psi \) the identity map, where \( 0 \) corresponds to the the identity map, where \( 0 \) denotes the constant zero function. The split of the affine coupling layers is fixed at \((|\frac{h}{2}|, D - |\frac{h}{2}|)\).

1 \times 1 convolution layers. We initialize the parameters of the neural networks by \( \mathcal{N}(0, \frac{1}{m}) \) where \( m \) is the number of parameters of each layer and \( \mathcal{N} \) is the normal distribution.

B.3 Model details: Penultimate layer networks

We initialize the parameter for each layer of \( \psi_d \) by \( U(-\sqrt{\frac{1}{m}}, \sqrt{\frac{1}{m}}) \), where \( m \) is the number of input features and \( U \) is the uniform distribution.

B.4 Training details

During the training of GCL, we fix the batch size at 32.

B.5 Compared methods details

\textit{TrAdaBoost.} As suggested in \textcite{Pardoe and Stone 2010}, we use the linear loss function and set the maximum number of internal boosting iterations at 30.

\textit{GDM.} We fix the number of sampling required for approximating the maximization in the generalization discrepancy at 200. This method presumes using hypothesis classes in a reproducing kernel Hilbert space (RKHS).

\textit{Copula.} For this model, the probabilistic model of non-parametric R-vine copula of depth 1 is used following \textcite{Lopez-paz et al. 2012}. Kernel density estimators with RBF kernel are used for estimating the marginal distributions and the copulas. The bandwidths of the RBF kernels are determined using the rule-of-thumb implemented as “normal-reference” in the \texttt{np} package of R language \textcite{Hayfield and Racine 2008}. The predictions are made by numerically aggregating the estimated conditional distribution over the interval \([\min(Y_i - 2\sigma, \max(Y_i + 2\sigma)] \) where \( \sigma \) denotes the square root of the unbiased variance of \( \{Y_i\}_{i=1}^{n_{src}} \). The aggregation is performed by discretizing the interval into a grid of 300 points. The level of the two-sample test is fixed at 0.05 for all combination of the two-sample tests following the experiment code of \textcite{Lopez-paz et al. 2012}. This method is a single-source domain adaptation method and we pool all source domain data for adaptation.

C Details and Proofs of Theorem[2]

Here, we detail the assumptions, the statement, and the proof of Theorem[2]

C.1 Notation

To make the proof self-contained, we first recall some general and problem-specific notation. In the notation here, we omit the domain identifiers from the distributions and the sample size, such as \textit{Tar} or \textit{Src}, because only the target domain data or their distributions appear in the proofs. The theorem holds regardless of how \( f \) is estimated as long as \( f \) is independent of the target domain data. In the proof, we extend the maximal discrepancy bound of U-statistics previously proved for the case of degree-2 in \textcite{Rejchel 2012}, to allow higher degrees.

General mathematical notation. We denote the set of natural numbers (resp. real numbers) by \( \mathbb{N} \) (resp. \( \mathbb{R} \)). For any \( N \in \mathbb{N} \), we define \( [N] := \{1, 2, \ldots, N\} \). We use \( \binom{a}{b} \) to denote the number of \( b \)-combinations of \( a \) elements. For a finite set \( A \), the notation \( \sum_{a \in A} \) denotes the operator to take an average over \( A \), i.e., \( \sum_{a \in A} h = \frac{1}{|A|} \sum_{a \in A} h(a) \). For a \( D \)-dimensional function \( h \), we denote its \( j \)-th dimension \( (j \in [D]) \) by suffixing \( h_j \). For a vector \( s \), we denote its \( j \)-th element by \( s^{(j)} \). We denote the Jacobian determinant of a differentiable function \( \psi \) at \( a \) by \( J\psi(a) := \det \frac{d\psi(a)}{da} \).
We denote the identity matrix by $I$ regardless of the size of the matrices when there is no ambiguity. For finite dimensional vectors, we denote the 2-norm by $\| \cdot \|_2$ and the 1-norm by $\| \cdot \|_1$. For square matrices, we denote the operator-2 norm by $\| \cdot \|_{op}$ and the operator-1 norm by $\| \cdot \|_{op(1)}$. We use $W^{k,p}$ to denote the Sobolev space (on $\mathbb{R}^D$) of order $k$ and define its associated norm by $\| h \|_{W^{k,p}} := \left( \sum_{|\alpha| \leq k} \| h^{(\alpha)} \|_{L^p} \right)^{1/p}$ where $\alpha$ is a multi-index and $h^{(\alpha)}$ denotes the partial derivative $\partial_{s_1}^{\alpha_1} \cdots \partial_{s_k}^{\alpha_k} h$ (Adams and Fournier, 2003, Paragraph 3.1). We let $\mathcal{S}_D$ be the degree-$D$ symmetric group. $\mathcal{S}_j^D := \{ \tau : [D] \to [j] \mid \tau \text{ is surjective} \}$ be the set of $j$-grouping of indices in $[D]$, and $\mathcal{J}_j^D := \{ \rho : [j] \to [n] \mid \rho \text{ is injective} \}$ be the set of all size-$j$ combinations (without replacement) of indices in $[n]$.

Distributions and expectations. We denote by $Q$ the set of all factorized distributions on $\mathbb{R}^D$ with absolutely continuous marginals. For a measure $P$, we denote its $j$-product measure by $P^j := P \otimes \cdots \otimes P$ (repeated $j$ times). We assume that all measures appearing in this proof are absolutely continuous with respect to the Lebesgue measure. The push-forward of a distribution $p$ by a function $h$ is denoted by $h_* p$. The expectation of a function $h$ with respect to measure $P$ is denoted by $\mathbb{E}_P[h]$ (if it exists) by abuse of notation. We also abuse the notation to use $\psi(s,P_1,\ldots,P)$ as the shorthand for $P^{D-1} \psi(s,S_2^D) := (s_{d_{j_{D-1}}} \cdots s_{d_{j_D}})$ where $\{S_d^D \}_{d=1}^{j_{D-1}} \sim P$. 

C.2 Problem setup

We denote the target domain distribution by $p$. We fix a hypothesis class $\mathcal{G}(\subset \{ g : \mathbb{R}^{D-1} \to \mathbb{R} \})$, and our goal is to find a $g \in \mathcal{G}$ such that the risk functional

$$R(g) := \int p(z) \ell(g(z)) \, dz$$

is small, where $\ell : \mathcal{G} \times \mathbb{R}^D \to \mathbb{R}_{\geq 0}$ is a loss function. We denote by $g^*$ a minimizer of $R$ (assuming it exists). To this end, we are given the training data $D := \{ Z_i \}_{i=1}^n \sim p$. Throughout, we assume $n \geq D$. To complement the smallness of $n$, we assume the existence of a generative mechanism. Concretely, we assume that there exists a diffeomorphism $f : \mathbb{R}^D \to \mathbb{R}^D$ such that $q := f_* p$ satisfies $q \in \mathcal{Q}$. With this transform, the original risk functional is also expressed as

$$R(g) = \int q(s) \ell(g,f(s)) \, ds.$$

As an estimator of $f$, we are given another diffeomorphism $\hat{f} : \mathbb{R}^D \to \mathbb{R}^D$ such that $\hat{f} \approx f$. With this $\hat{f}$, the proposed method converts the dataset $D$ by $S := \hat{f}(Z_i)$. We can regard $\hat{D} := \{ S_i \}_{i=1}^n \sim q$, where $q := (\hat{f}^{-1} \circ f)_* q$. We use $\hat{Q}$ (resp. $\hat{Q}$) to denote the probability measure corresponding to the density $q$ (resp. $\hat{q}$). This conversion results in the relation:

$$\hat{q}(s) = q(f^{-1} \circ \hat{f})(s) \left| (Jf^{-1} \circ \hat{f})(s) \right|.$$ 

As a candidate hypothesis $g \in \mathcal{G}$, the proposed method selects a minimizer $\hat{g} \in \mathcal{G}$ of the proposed risk estimator $\hat{R}$ defined as

$$\hat{R}(g) := \frac{1}{n^{D}} \sum_{(i_1,\ldots,i_D) \in [n]^{D}} \ell(g,\hat{f}(s_{i_1}^{(1)},\ldots,s_{i_D}^{(D)})). \tag{5}$$

In the proof, we evaluate its concentration around the expectation $\bar{R}(g) := \mathbb{E}_\hat{D} \hat{R}(g)$. We use $\mathbb{E}_\hat{D}$ to denote the expectation with respect to $\hat{D}$. Let $\bar{g}$ denote a hypothesis which minimizes $\bar{R}(g)$ (assuming it exists).

In what follows, for notational simplicity, we define the $D$-variate symmetric function $\hat{\ell}$ as

$$\hat{\ell}(s_1,\ldots,s_D) = \sum_{\pi \in \mathcal{S}_D} \ell(g,\hat{f}(s_{\pi(1)}^{(1)},\ldots,s_{\pi(D)}^{(D)}),$$

where $\sum_{\pi \in \mathcal{S}_D}$ indicates an averaging operation over all permutations (without replacement) of $[D]$. We use $\hat{E}_n$ to denote the sample average operator with respect to $D$ or $\hat{D}$, depending on the context.
C.3 Assumptions

Assumption 2 (The underlying density function is bounded and Lipschitz continuous). Assume

\[ B_q := \sup_{s \in \mathbb{R}^d} q(s) < \infty, \quad L_q := \sup_{s_1 \neq s_2} \frac{|q(s_1) - q(s_2)|}{\|s_1 - s_2\|} < \infty. \]

Assumption 3 (\(f^{-1}\) is Lipschitz continuous and Hölder continuous). We assume \(f^{-1} \in C^{1,1}\) where \(C^{1,1}\) is the \((1, 1)\)-Hölder space (Adams and Fournier, 2003, Paragraph 1.29) and

\[ L_{f^{-1}} := \sup_{z_1 \neq z_2} \frac{|f^{-1}(z_1) - f^{-1}(z_2)|}{\|z_1 - z_2\|} < \infty. \]

Assumption 4 (Bounded derivatives of \(f\) and \(f^{-1}\)). Assume that

\[ B_{df} := \sup_{s \in \mathbb{R}^d} \left\| \frac{df}{ds}(s) \right\|_{\infty} < \infty, \quad B_{df^{-1}} := \sup_{z \in \mathbb{R}^d} \left\| \frac{df^{-1}}{dz}(z) \right\|_{\infty} < \infty. \]

where \(\|\|_{\infty}\) denotes the maximum absolute value of the elements of a matrix.

Assumption 5 (Loss function is bounded and uniformly Lipschitz continuous in \(Z\)). The considered loss function takes values in a bounded interval:

\[ \ell : \mathcal{G} \times Z \rightarrow [0, B_\ell], \]

where \(0 < B_\ell < \infty\). Also assume

\[ L_{\ell, \Phi} := \sup_{g \in \mathcal{G}} \sup_{z_1 \neq z_2} \left| \ell(g, z_1) - \ell(g, z_2) \right| \frac{1}{\|z_1 - z_2\|} < \infty. \]

Assumption 6 (Estimated feature extractor). Assume \(\hat{f}\) is independent of \(D\) and that \(f_j - \hat{f}_j \in W^{1, d}\) for all \((j, d) \in [D] \times [D]\).

Although \(\hat{f}\) and \(f\) are assumed to be diffeomorphisms in the classical sense (implying that they are strongly differentiable), we introduce the Sobolev space because we want to measure their difference and their difference of derivatives in terms of integration.

Assumption 7 (Entropic condition: Euclidean class (Sherman, 1994)). The function class \(\Phi := \{\tilde{g} : g \in \mathcal{G}\} \) is Euclidean for the envelope \(F\) and constants \(A\) and \(V\) (Sherman, 1994), i.e., if \(\mu\) is a measure for which \(\mu F^2 < \infty\), then

\[ D(t, d_\mu, \Phi) \leq At^{-V}, \quad 0 < t \leq 1, \]

where \(d_\mu\) is the pseudo metric defined by

\[ d_\mu(\phi_1, \phi_2) := \left[ \mu |\phi_1 - \phi_2|^2 / \mu F^2 \right]^{1/2} \]

for \(\phi_1, \phi_2 \in \Phi\), and \(D(t, d_\mu, \Phi)\) denotes the packing number of \(\Phi\) with respect to the pseudometric \(d_\mu\) and radius \(t\). Without loss of generality, we take the envelope \(F\) such that \(F(\cdot) \leq B_\ell\).

Assumption 8. The hypothesis class \(\mathcal{G}\) is expressive enough so that the model approximation error does not expand due to \(\hat{f}\), i.e.,

\[ \inf_{g \in \mathcal{G}} \tilde{R}(g) \leq \inf_{g \in \mathcal{G}} R(g) \]

The following complexity measure of \(\mathcal{G}\), which is a version of Rademacher complexity for our problem setting, is used to state the theorem.

**Definition 1** (Effective Rademacher complexity). Define

\[ \mathcal{R}(\mathcal{G}) := \frac{1}{n} \mathbb{E}_{\tilde{R}} \left[ \sup_{g \in \mathcal{G}} \left| \sum_{i=1}^{n} \sigma_i \mathbb{E}_{S_i, \ldots, S_{D}^{i.d.}} \left[ \tilde{R}(S_i, S_2', \ldots, S_D') \right] \right| \right] \]

where \(\{\sigma_i\}_{i=1}^{n}\) are independent uniform sign variables and \(S_2', \ldots, S_D^{i.d.} \sim Q\) are independent of all other random variables.

We provide the definition of the ordinary Rademacher complexity in Section C.8 and make a comparison of the two complexity measures in terms of how they depend on the input dimensionality.
C.4 Theorem statement

Our goal is to prove the following theorem. This is a detailed version of the theorem appearing in the main body of the paper.

**Theorem 3** (Excess risk bound). Assume Assumptions 2, 3, 5, 6, 7, and 8.

Then for arbitrary $\delta, \delta' \in (0, 1)$, we have with probability at least $1 - (\delta + \delta')$,

$$R(\hat{g}) - R(g^*) \leq C \sum_{j=1}^{D} \left\| f_j - \hat{f}_j \right\|_{W^{1.1}} + 4D\mathcal{R}(G) + 2DB_{l} \sqrt{\frac{\log 2/\delta}{2n}} + \kappa_1(\delta', n) + DB_{l} B_{q} \kappa_2(f - \hat{f}).$$

where

$$C := B_{q} L_{\ell_{0}} + DB_{l}(L_{q} L_{f-1} + B_{q} DC_{1}'),$$

$$C_{1}' := (D + 1)^{3/2} \left( B'_{1} \sum_{k=1}^{D} \left\| f_k^{-1} \right\|_{C^{1.1}} \right) + B'_{1},$$

$$\kappa_1(\delta', n) = \mathcal{O}(n^{-1})/\delta' + \mathcal{O}(n^{-1}),$$

$$\kappa_2(f - \hat{f}) = \sum_{d=2}^{D} \left( \frac{D}{d} \right) C_{d} \sum_{j=1}^{D} \left\| f_j - \hat{f}_j \right\|_{W^{1.1}}^{d}.$$

and $C_{d}^{1}(d = 1, \ldots, D)$ are constants determined in Lemma 11.

**Proof of Theorem 3**. By adding and subtracting terms, we have

$$R(\hat{g}) - R(g^*) = (R - \tilde{R}(\hat{g})) + \tilde{R}(\hat{g}) - \tilde{R}(\tilde{g}) + \tilde{R}(\tilde{g}) - R(g^*).$$

(A) Approximation error  (B) Pseudo estimation error  (C) Additional model misspecification error

Applying Lemma 11 to (A), Lemma 2 to (B), and Assumption 8 to (C), we obtain the assertion. \qed

As it can be seen from the proof above, Theorem 3 is proved in two parts, each corresponding to the two lemmas below. The first lemma evaluates the approximation error which reflects the fact that we are approximating $f$ by $\hat{f}$.

**Lemma 1** (Approximation error bound). Given Assumptions 2, 3, 5, 6, and 7 we have

$$(R - \tilde{R}(\hat{g})) \leq C \sum_{j=1}^{D} \left\| f_j - \hat{f}_j \right\|_{W^{1.1}} + DB_{l} B_{q} \kappa_2(f - \hat{f}).$$

where $C$ and $\kappa_2(f - \hat{f})$ are

$$C := B_{q} L_{\ell_{0}} + DB_{l}(L_{q} L_{f-1} + B_{q} DC_{1}'),$$

$$\kappa_2(f - \hat{f}) := \sum_{d=2}^{D} \left( \frac{D}{d} \right) C_{d} \sum_{j=1}^{D} \left\| f_j - \hat{f}_j \right\|_{W^{1.1}}^{d}.$$

and $C_{d}^{1}(d = 1, \ldots, D)$ are constants determined in Lemma 11.

The second lemma evaluates the pseudo estimation error which reflects the fact that we rely on a finite sample to approximate the underlying distribution.

**Lemma 2** (Pseudo estimation error bound). Assume that Assumptions 2 and 5 hold. Let the Rademacher complexity be defined as Definition 4. Then for any $\delta, \delta' \in (0, 1)$, we have with probability at least $1 - (\delta + \delta')$ that

$$\tilde{R}(\hat{g}) - \tilde{R}(\tilde{g}) \leq 4Dw_{D}\mathcal{R}(G) + 2DB_{l}w_{D} \sqrt{\frac{\log 2/\delta}{2n}} + 2w_{D}(D - 1) \sum_{j=2}^{D} \frac{C_{j}}{\delta' n^{-j/2}} + 4B_{l} \sum_{j=1}^{D-1} w_{j},$$

where $\{w_{j}\}_{j=1}^{D}$ are universal constants determined in Lemma 3 and $\{C_{j}\}_{j=2}^{D}$ are constants determined in Lemma 6.

Note that $w_{j} = \mathcal{O}(n^{-(D-j)})$ and $w_{D} = \frac{n(n-1)\cdots(n-D+1)}{n^{D}} < 1$. 

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In what follows, we first present some basic facts in Section C.5 and provide the proofs for the lemmas. We provide the proof of Lemma 1 in Section C.7 and that of Lemma 2 in Section C.6.

C.5 V-statistic and U-statistic

The theoretical analysis is performed by interpreting the proposed risk estimator Eq. (5) as a V-statistic (explained shortly). The proofs will be based on applying the following facts in order:

1. V-statistic can be represented as a weighted average of U-statistics with degrees from 1 to $D$, and only the degree-$D$ term is the leading term.
2. The degree-$D$ term is again decomposed into a degree-1 U-statistic and a set of degenerate U-statistics.
3. The degree-1 U-statistic is an i.i.d. sum admitting a Rademacher complexity bound.
4. The degenerate terms concentrate around zero following an exponential inequality under appropriate entropy conditions.

To consolidate the strategy given above, we describe what are V- and U-statistics, and how they relate to each other. These estimators emerge when we allow re-using the same data point repeatedly from a single sample to estimate a function which takes multiple data points.

**V-statistic.** For a given regular statistical functional of degree $D$ (Lee, 1990):

$$\hat{Q}^D \hat{\ell} := \int \hat{\ell}(s_1, \ldots, s_D)\hat{q}(s_1) \cdots \hat{q}(s_D)ds_1 \cdots ds_D,$$

its associated von-Mises statistic (V-statistic) is the following quantity (Lee, 1990):

$$V^D_n \hat{\ell} := \frac{1}{n^D} \sum_{i_1=1}^{n} \cdots \sum_{i_D=1}^{n} \hat{\ell}(S_{i_1}, \ldots, S_{i_D}).$$

Note that Eq. 6 does not coincide with the expectation of $V^D_n \hat{\ell}$ in general, i.e., the V-statistic is generally not an unbiased estimator. However, it is known to be a consistent estimator of Eq. (6) (Lee, 1990).

**U-statistic.** Similarly, for a $j$-variate symmetric and integrable function $h(x_1, \ldots, x_j)$, its corresponding U-statistic (Lee, 1990) of degree $j$ is

$$U^j_n h := \sum_{\rho \in \mathcal{G}^j} h(s_{\rho(1)}, \ldots, s_{\rho(j)}).$$

The V- and U-statistics are generalizations of the sample mean (which is the U- and V-statistics of degree 1). The important difference from the sample mean in higher degrees is that the summands may not be independent. To deal with the dependence, the following standard decompositions have been developed (Lee, 1990).

**Lemma 3 (Decomposition of a V-statistic (Lee, 1990)).** A V-statistic can be expressed as a sum of U-statistics of degrees from 1 to $D$ (Lee, 1990, Section 4.2, Theorem 1):

$$V^D_n \hat{\ell} = \sum_{j=1}^{D} w_j U^j_n \tilde{\ell}(j)$$

where the weights $w_j$ and $j$-variate functions $\tilde{\ell}(j)$ are

$$w_j := \frac{1}{n^D} |\mathcal{G}^D_j| \binom{n}{j}, \quad \tilde{\ell}(j)(s_1, \ldots, s_j) := \sum_{\tau \in \mathcal{G}^D_j} \hat{\ell}(s_{\tau(1)}, \ldots, s_{\tau(D)}).$$

**Proof.** See (Lee, 1990, Section 4.2, Theorem 1 (p.183)).

**Remark 1.** The weights $\{w_j\}_{j=1}^{D}$ satisfy $\sum w_j = 1$ (Lee, 1990, Section 4.2, Theorem 1 (p.183)). We can also find the order of $w_j$ with respect to $n$ as:

$$w_D = \frac{1}{n^D} |\mathcal{G}^D_D| \binom{n}{D} = \frac{n(n-1) \cdots (n-D+1)}{n^D} = O(1), \quad w_j = O(n^{-(D-j)}), \quad \tilde{\ell}(D) = \hat{\ell}.$$
**Lemma 4** (Hoeffding decomposition of a U-statistic [Sherman, 1994, p.449]). A U-statistic with a symmetric kernel \( \psi \) can be decomposed as a sum of U-statistics of degrees from 1 to \( D \) as

\[
U_n^D \psi - \mathbb{E}_D U_n^D \psi = \sum_{j=1}^D U_j \psi_j \\
= \hat{\mathbb{E}}_n \psi_1 + \sum_{j=2}^D U_j \psi_j
\]

where \( \{ \psi_j \}_{j=1}^D \) are \( j \)-variate, symmetric and degenerate functions. Note that \( \mathbb{E}_D U_n^D \psi = \hat{Q}^D \psi \). Here, a \( j \)-variate symmetric function \( \psi_j \) is said degenerate when

\[
\forall s_2, \ldots, s_j, \quad \psi_j(\hat{Q}, s_2, \ldots, s_j) = 0.
\]

Specifically, \( \psi_1 \) is

\[
\psi_1(s) = \psi(s, \hat{Q}, \ldots, \hat{Q}) + \cdots + \psi(\hat{Q}, \ldots, s, \hat{Q}) - D \hat{Q}^D \psi
\]

\[
= D \cdot (\psi(s, \hat{Q}, \ldots, \hat{Q}) - \hat{Q}^D \psi) \quad \text{(by symmetry).}
\]

For further details, see [Sherman, 1994, p.449]. Note that in [Sherman, 1994, p.449], Eq. (7) is written using \( \hat{Q}^D \psi \) in place of \( \mathbb{E}_D U_n^D \psi \). This is because

\[
\mathbb{E}_D U_n^D \psi = U_n^D \mathbb{E}_D \psi = U_n^D \hat{Q}^D \psi = \hat{Q}^D \psi
\]

holds by linearity and symmetry.

**Remark 2** (Connecting the lemmas to Section C.6). It can be easily checked by definition that the proposed risk estimator Eq. (5) takes the form of a V-statistic: \( \hat{R}(g) = V_n^D \hat{\ell} \) for each \( g \in G \). Let us denote \( \hat{\ell}^* (s) := \hat{\ell}(s, \hat{Q}, \ldots, \hat{Q}) \). Then \( \mathbb{E}_D \hat{\ell}^* = \hat{Q}^D \hat{\ell} \) holds by definition. Substituting these into Eq. (8), we have that Eq. (7) applied to \( \psi = \hat{\ell} \) is equivalent to

\[
U_n^D \hat{\ell} - \mathbb{E}_D U_n^D \hat{\ell} = D \cdot (\hat{\mathbb{E}}_n \hat{\ell}^* - \mathbb{E}_D \hat{\ell}^*) + \sum_{j=2}^D U_j \hat{\ell}_j.
\]

where \( \{ \hat{\ell}_j \}_{j=2}^D \) are symmetric degenerate functions. In Section C.6 we first decompose \( \hat{R}(g) \) into a sum of U-statistics. After such conversion, we take a closer look at the leading term, \( \mathbb{E}_n \hat{\ell}^* \).

### C.6 Proof of pseudo estimation error bound

(Proof of Lemma 2). First, we have

\[
\hat{R}(\hat{g}) - \hat{R}(\tilde{g}) = \hat{R}(\hat{g}) - \hat{R}(\tilde{g}) + \hat{R}(\tilde{g}) - \tilde{R}(\tilde{g}) \leq \hat{R}(\hat{g}) - \hat{R}(\tilde{g}) + R(\tilde{g}) - \tilde{R}(\tilde{g})
\]

\[
\leq 2 \sup_{g \in G} \left| \hat{R}(g) - \tilde{R}(g) \right|.
\]
Now the right-most expression can be decomposed as
\[
\sup_{g \in \mathcal{G}} |\hat{R}(g) - \tilde{R}(g)| = \sup_{g \in \mathcal{G}} |V_n^D \tilde{\ell} - \mathbb{E}_B V_n^D \tilde{\ell}|
\]
\[
\leq w_D \sup_{g \in \mathcal{G}} \left| U_n^D \tilde{\ell} - \mathbb{E}_B U_n^D \tilde{\ell} \right| + \sum_{j=1}^{D-1} w_j \sup_{g \in \mathcal{G}} \left| U_n^j \tilde{\ell}^{(j)} - \mathbb{E}_B U_n^j \tilde{\ell}^{(j)} \right| \quad (\because \text{Lemma 3})
\]
\[
\leq w_D \sup_{g \in \mathcal{G}} \left| U_n^D \tilde{\ell} - \mathbb{E}_B U_n^D \tilde{\ell} \right| + 2B_{t} \sum_{j=1}^{D-1} w_j
\]
\[
\leq w_D \left( \sup_{g \in \mathcal{G}} |\hat{E}_n \tilde{\ell}| + \sum_{j=2}^{D} \sup_{g \in \mathcal{G}} |U_n^j \tilde{\ell}_j| \right) + 2B_{t} \sum_{j=1}^{D-1} w_j \quad (\because \text{Lemma 4})
\]
\[
= w_D \left( \sup_{g \in \mathcal{G}} |\hat{E}_n \tilde{\ell}| + \sum_{j=2}^{D} \sup_{g \in \mathcal{G}} |U_n^j \tilde{\ell}_j| \right) + 2B_{t} \sum_{j=1}^{D-1} w_j
\]

where \( \tilde{\ell}_j \) are symmetric degenerate functions and \( \tilde{\ell}^* \) is defined as in Remark 2. Applying Lemma 3 to the first term and Lemma 4 to the second term with the union bound, we obtain the assertion. \( \square \)

In the last part of the proof we used the following lemmas. Because the leading term is an i.i.d. sum, the following Rademacher complexity bound can be proved.

**Lemma 5 (U-process bound: the leading term).** Assume Assumption 2 holds. Then, we have with probability at least \( 1 - \delta \),
\[
\sup_{g \in \mathcal{G}} |\hat{E}_n (\tilde{\ell}^* - \mathbb{E}_B \tilde{\ell}^*)| \leq 2\mathcal{R}(\mathcal{G}) + B_{t} \sqrt{\frac{\log(2/\delta)}{2n}},
\]
where \( \mathcal{R} \) is defined in Definition 7.

**Proof.** Applying the standard one-sided Rademacher complexity bound based on McDiarmid’s inequality (Mohri et al. 2012 Theorem 3.1) twice with the union bound, we obtain the lemma. \( \square \)

The other terms than the leading term are degenerate U-statistics, hence the following holds under appropriate entropy assumptions.

**Lemma 6 (U-process bound: degenerate terms (Sherman [1994 Corollary 7])).** Assume Assumption 2. Then for each \( j = 2, \ldots, D \), there exist constants \( C_j \) such that for any \( \delta \in (0, 1) \), we have with probability at least \( 1 - \delta'/(D - 1) \),
\[
\sup_{g \in \mathcal{G}} |U_n^j \tilde{\ell}_j| \leq \frac{(D - 1)}{\delta'} C_j n^{-j/2}
\]

where \( C_j \) depends only on \( A, V, \) and \( B_{t} \).

**Proof.** The proof follows a similar path as that of Sherman [1994 Corollary 7], but we provide more explicit expressions to inspect the order with respect to \( n \). Let \( \Phi^{(j)}_{g, f} := \{ f_j : g \in \mathcal{G} \} \). Then \( \Phi^{(j)}_{g, f} \) is Euclidean for an envelope \( F_j \) satisfying \( \hat{Q}^j F_j^2 < \infty \) by Lemma 6 in Sherman [1994] and Assumption 7. In addition, \( \Phi^{(j)}_{g, f} \) is a set of functions degenerate with respect to \( \hat{Q} \). Without loss of generality, we can take \( F_j \) such that \( F_j \leq B_{t} \). Similarly to the proof of Sherman [1994 Main Corollary] with \( p = 1 \) in their notation to obtain
\[
\mathbb{E}_D \sup_{g \in \mathcal{G}} |n^{j/2} U_n^j \tilde{\ell}_j| \leq \Gamma A^{1/2mp} (\hat{Q}^j F_j^2)^{(\epsilon+\alpha)/2} \leq \Gamma A^{1/2mp} (B_{t})^{\epsilon+\alpha} =: C_j
\]

where \( \Gamma \) is a universal constant (Sherman [1994 Main Corollary]), \( \epsilon \in (0, 1) \) and \( m \) are chosen to satisfy \( 1 - V/2m > 1 - \epsilon \), and \( \alpha = 1 - V/2m \). By applying Markov inequality, we have for arbitrary \( u > 0 \),
\[
\mathbb{P}_D \left( \sup_{g \in \mathcal{G}} |n^{j/2} U_n^j \tilde{\ell}_j| > u \right) \leq \frac{C_j}{u},
\]

where \( C_j \) depends on \( A, V, \) and \( B_{t} \).
where $\mathbb{P}_D(E)$ denotes the probability of the event $E$ with respect to $\hat{D}$. Equating the right hand side with $\delta^\prime/(D-1)$ and solving for $u$, we obtain the result.

\[\]

**C.7 Proof of approximation error bound**

(Proof of Lemma 7). Due to Lemma 5 we have

\[
\sup_{g \in \mathcal{G}} \left( R(g) - \bar{R}(g) \right) = \sup_{g \in \mathcal{G}} \left( R(g) - \mathbb{E}_D U_n^D \hat{\ell} \right)
\]

\[
= \sup_{g \in \mathcal{G}} \left( \sum_{j=1}^{D} w_j (R(g) - \mathbb{E}_D U_n^{j} \hat{\ell}(j)) \right)
\]

\[
\leq w_D \sup_{g \in \mathcal{G}} \left( R(g) - \mathbb{E}_D U_n^{D} \hat{\ell}(D) \right) + 2B_t \sum_{j=1}^{D-1} w_j \mathbb{O}(n^{-(D-j)})
\]

\[
\leq w_D \sup_{g \in \mathcal{G}} \left( R(g) - \mathbb{E}_D U_n^{D} \hat{\ell}(D) \right) + 2B_t \mathbb{O}(n^{-1})
\]

By applying Lemmas 7 (with $j = D$), we obtain

\[
\sup_{g \in \mathcal{G}} \left( R(g) - \mathbb{E}_D U_n^{D} \hat{\ell}(D) \right) \leq \sup_{g \in \mathcal{G}} \left\| \ell(f(g, \cdot)) - \ell(g, \hat{f}(\cdot)) \right\|_{L^1(g)} + DB_t \|q - \bar{q}\|_{L^1}.
\]

The right-hand side can be further bounded by applying Lemmas 9 and 8 by

\[
B_q L_{\ell_q} \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,1}} + DB_t \left( (L_q L_f^{-1} + B_q DC^1_q) \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,1}} + B_q \kappa_2(f - \hat{f}) \right)
\]

\[
\leq (B_q L_{\ell_q} + DB_t (L_q L_f^{-1} + B_q DC^1_q)) \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,1}} + DB_t B_q \kappa_2(f - \hat{f})
\]

and hence the assertion of the lemma.

The above proof combined three approximation bounds, which are shown in the following lemmas. The following lemma reduces the difference in the expectation of U-statistic into the differences in the loss function and the density function. Although we apply the following Lemma 7 only with $j = D$, we prove its general form for $j \in [D]$.

**Lemma 7** (Approximation bound for U-statistic of degree-$j$). Fix $j \in [D]$. Assume Assumption 2. Then we have for any $g \in \mathcal{G}$,

\[
R(g) - \mathbb{E}_D U_n^j \bar{\ell}(j) \leq \left\| \ell(g, f(\cdot)) - \ell(g, \hat{f}(\cdot)) \right\|_{L^1(g)} + jB_t \|q - \bar{q}\|_{L^1}
\]

**Proof.** Let us define a $D$-variate function $\ell^j$ and a $j$-variate function $\ell^{(j)}$ (similarly to $\hat{\ell}$ and $\bar{\ell}(j)$, respectively) by

\[
\ell^j(s_1, \ldots, s_D) := \sum_{\tau \in \mathcal{G}_D} \ell(g, f(s^{(1)}_{\tau(1)}, \ldots, s^{(D)}_{\tau(D)})).
\]

\[
\ell^{(j)}(s_1, \ldots, s_j) := \sum_{\tau \in \mathcal{G}_j} \ell^j(s^{(1)}_{\tau(1)}, \ldots, s_{\tau(D)}).
\]
Then, recalling $Q \in Q$, we can show $R(g) = Q^n(\hat{U}_n^j \hat{\ell}(j))$ because

$$Q^n(\hat{U}_n^j \hat{\ell}(j)) = Q^n \left( \sum_{\rho \in J_n} \ell^{(j)}(S_{\rho(1)}, \ldots, S_{\rho(j)}) \right)$$

$$= Q^n \left( \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} \ell(g, f(S_{\rho(1)}^{(1)}, \ldots, S_{\rho(D)}^{(D)})) \right)$$

$$= \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} Q^n \ell(g, f(S_{\rho(1)}^{(1)}, \ldots, S_{\rho(D)}^{(D)}))$$

$$= \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} Q[\ell(g, f(S^{(1)}, \ldots, S^{(D)}))] \ (:: Q \in Q)$$

$$= \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} R(g) = R(g).$$

Combining this expression with Lemma 3

$$R(g) - \mathbb{E}_D \hat{U}_n^j \hat{\ell}(j) = Q^n(\hat{U}_n^j \hat{\ell}(j)) - \hat{Q}^n(\hat{U}_n^j \hat{\ell}(j))$$

$$= \frac{Q^n(\hat{U}_n^j \hat{\ell}(j) - \hat{U}_n^j \hat{\ell}(j))}{A} + \frac{(Q^n - \hat{Q}^n)(\hat{U}_n^j \hat{\ell}(j))}{B}$$

Now, $A$ can be bounded from above as

$$A = Q^n(\hat{U}_n^j \hat{\ell}(j) - \hat{U}_n^j \hat{\ell}(j))$$

$$= \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} Q^n(\ell(g, f(S_{\rho(1)}^{(1)}, \ldots, S_{\rho(D)}^{(D)})) - \ell(g, \hat{f}(S_{\rho(1)}^{(1)}, \ldots, S_{\rho(D)}^{(D)})))$$

$$= \sum_{\rho \in J_n} \sum_{\tau \in \Theta_n} \sum_{\pi \in \Theta_D} Q[\ell(g, f(S^{(1)}, \ldots, S^{(D)})) - \ell(g, \hat{f}(S^{(1)}, \ldots, S^{(D)}))] \ (:: Q \in Q)$$

$$\leq \left\| \ell(g, f(\cdot)) - \ell(g, \hat{f}(\cdot)) \right\|_{L^1(g)}$$

Then recalling Assumption 3 we can bound $B$ from above as

$$B = (Q^n - \hat{Q}^n)(\hat{U}_n^j \hat{\ell}(j)) = (Q^n - \hat{Q}^n) \left( \sum_{\rho \in J_n} \hat{\ell}(j)(S_{\rho(1)}, \ldots, S_{\rho(j)}) \right)$$

$$= \sum_{\rho \in J_n} (Q^n - \hat{Q}^n) \left( \hat{\ell}(j)(S_{\rho(1)}, \ldots, S_{\rho(j)}) \right) = (Q^j - \hat{Q}^j)(\hat{\ell}(j)(S_1, \ldots, S_j)) \ (:: \text{symmetry})$$

$$\leq B \ell \int \prod_{i=1}^{j} q(s_i) - \prod_{i=1}^{j} \hat{q}(s_i) \ |ds_1 \cdots ds_j$$

$$= B \ell \int \sum_{i=1}^{j} q(s_1) \cdots q(s_{i-1}) \cdot (q(s_i) - \hat{q}(s_i)) \cdot \hat{q}(s_{i+1}) \cdots \hat{q}(s_j) \ |ds_1 \cdots ds_j$$

$$\leq B \ell \int \sum_{i=1}^{j} q(s_1) \cdots q(s_{i-1}) \cdot |q(s_i) - \hat{q}(s_i)| \cdot \hat{q}(s_{i+1}) \cdots \hat{q}(s_j) \ |ds_1 \cdots ds_j$$

$$= B \ell \int \sum_{i=1}^{j} |q(s_i) - \hat{q}(s_i)| \ |ds_i = B \ell \cdot j \|q - \hat{q}\|_{L^1},$$

which proves the assertion. \qed
Now the following lemmas bound each approximation terms in terms of the difference between \( f \) and \( \hat{f} \).

**Lemma 8** (Loss difference approximation). Assume Assumption 5\(^\star\). Then we have for any \( g \in \mathcal{G} \),

\[
\left\| \ell(g, f(\cdot)) - \ell(g, \hat{f}(\cdot)) \right\|_{L^1(q)} \leq B_q L_{\ell_\mathcal{G}} \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}}
\]

**Proof.**

\[
\left\| \ell(g, f(\cdot)) - \ell(g, \hat{f}(\cdot)) \right\|_{L^1(q)} = \int \left| \ell(g, f(s)) - \ell(g, \hat{f}(s)) \right| q(s) \, ds \\
\leq B_q \int L_{\ell_\mathcal{G}} \left\| f(s) - \hat{f}(s) \right\|_{\ell^2} \, ds \\
\leq B_q L_{\ell_\mathcal{G}} \int \left\| f(s) - \hat{f}(s) \right\|_{\ell^1}, \, ds \leq B_q L_{\ell_\mathcal{G}} \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}}.
\]

**Lemma 9** (Density difference approximation). Assume Assumptions 2, 3, and 4. Then we have

\[
\| q - \tilde{q} \|_{L^1} \leq (L_df_{f-1} + B_q DC_1) \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}} + B_q \kappa_2(f - \hat{f})
\]

where \( C_1^q \) and \( \kappa_2(f - \hat{f}) \) are defined as in Lemma 11.

**Proof.** Since \( \tilde{q}(s) = q(f^{-1} \circ \hat{f}(s)) \left( (Jf^{-1} \circ \hat{f})(s) \right) \), we have

\[
\left\| q - \tilde{q} \right\|_{L^1} = \int \left| q(s) - q(f^{-1} \circ \hat{f}(s)) \left( (Jf^{-1} \circ \hat{f})(s) \right) \right| \, ds \\
\leq \int \left| q(s) - q(f^{-1} \circ \hat{f}(s)) \right| ds + \int q(f^{-1} \circ \hat{f}(s)) \left| 1 - \left( (Jf^{-1} \circ \hat{f})(s) \right) \right| ds \\
\leq \int \left| q(s) - q(f^{-1} \circ \hat{f}(s)) \right| ds + B_q \int \left| 1 - (Jf^{-1} \circ \hat{f})(s) \right| ds
\]

where the last line follows from the triangle inequality. Applying Lemma 10 to (A) and Lemma 11 to (B) yields the assertion.

**Lemma 10.** Assume Assumptions 2 and 3. Then,

\[
\int \left| q(s) - q(f^{-1} \circ \hat{f}(s)) \right| ds \leq L_df_{f-1} \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}}
\]

**Proof.** We have

\[
\int \left| q(s) - q(f^{-1} \circ \hat{f}(s)) \right| ds = \int \left| q(f^{-1} \circ f(s)) - q(f^{-1} \circ \hat{f}(s)) \right| ds \\
\leq L_d L_{f-1} \int \left\| f(s) - \hat{f}(s) \right\|_{\ell^2} \, ds \leq L_d L_{f-1} \int \left\| f(s) - \hat{f}(s) \right\|_{\ell^1} \, ds \\
\leq L_d L_{f-1} \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}}.
\]
Lemma 11 (Jacobian difference approximation). Assume Assumptions 2 and 4. Then,

\[
\int \left| 1 - (J f^{-1} \circ \hat{f})(s) \right| ds \leq DC'_d \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,1}} + \kappa_2(f - \hat{f}),
\]

where

\[
C'_d := (D + 1)^{2d-2} \left( (B_f^\infty)^d \left( \sum_{k=1}^D \left\| f_k^{-1} \right\|_{C^{1,1}} \right)^d + (B_f^\infty)^d \right),
\]

\[
\kappa_2(f - \hat{f}) := \sum_{d=2}^D \binom{D}{d} C'_d \sum_{j=1}^D \left\| f_j - \hat{f}_j \right\|_{W^{1,d}}^d.
\]

Proof. Applying Lemma 12 with \( A := (J f^{-1} \circ f)(s) = I \), we obtain

\[
\int \left| 1 - (J f^{-1} \circ \hat{f})(s) \right| ds = \int \left| (J f^{-1} \circ f)(s) - (J f^{-1} \circ \hat{f})(s) \right| ds
\]

\[
\leq \int \sum_{d=1}^D \binom{D}{d} \left\| \frac{df^{-1} \circ f(s) - df^{-1} \circ \hat{f}(s)}{ds} \right\|_{op}^d ds.
\]
Now, each term in the integrand can be bounded from above as

\[
\left\| \frac{df^{-1} \circ f}{ds}(s) - \frac{df^{-1} \circ \hat{f}}{ds}(s) \right\|_{op} \\
\leq \left\| \left( \frac{df^{-1}}{dz}(f(s)) \right) \left( \frac{df}{ds}(s) \right) - \left( \frac{df^{-1}}{dz}(\hat{f}(s)) \right) \left( \frac{df}{ds}(s) \right) \right\|_{op} \\
\leq \left\| \frac{df^{-1}}{dz}(f(s)) - \frac{df^{-1}}{dz}(\hat{f}(s)) \right\|_{op} \left\| \frac{df}{ds}(s) \right\|_{op} + \left\| \frac{df^{-1}}{dz}(\hat{f}(s)) \right\|_{op} \left\| \frac{df}{ds}(s) - \frac{df}{ds}(s) \right\|_{op} \\
\leq \left\| \frac{df^{-1}}{dz}(f(s)) - \frac{df^{-1}}{dz}(\hat{f}(s)) \right\|_{op} \left\| D \cdot \left\| \frac{df}{ds}(s) \right\|_{\infty} \right\| + \left\| \frac{df^{-1}}{dz}(\hat{f}(s)) \right\|_{op} \left\| \frac{df}{ds}(s) - \frac{df}{ds}(s) \right\|_{op} \\
\leq DB_{df}^\infty \sqrt{D} \left\| \frac{df^{-1}}{dz}(f(s)) - \frac{df^{-1}}{dz}(\hat{f}(s)) \right\|_{op(1)} + DB_{df}^{\infty - 1} \sqrt{D} \left\| \frac{df}{ds}(s) - \frac{df}{ds}(s) \right\|_{op(1)} \\
= D^2 B_{df}^{\infty} \max_{k \in [D]} \sum_{j=1}^{D} \left| \frac{\partial f_j^{-1}}{\partial s_k}(f(s)) - \frac{\partial f_j^{-1}}{\partial s_k}(\hat{f}(s)) \right| + D^2 B_{df}^{\infty - 1} \max_{k \in [D]} \sum_{j=1}^{D} \left| \frac{\partial f_j}{\partial s_k}(s) - \frac{\partial \hat{f}_j}{\partial s_k}(s) \right| \\
\leq D^2 B_{df}^{\infty} \max_{k \in [D]} \sum_{j=1}^{D} \left\| f_j^{-1} \right\|_{C^{1,1}} \left\| f(s) - \hat{f}(s) \right\|_{C^1} + D^2 B_{df}^{\infty - 1} \sum_{k=1}^{D} \sum_{j=1}^{D} \left| \frac{\partial f_j}{\partial s_k}(s) - \frac{\partial \hat{f}_j}{\partial s_k}(s) \right| \\
\leq D^2 B_{df}^{\infty} \left( \sum_{j=1}^{D} \left\| f_j^{-1} \right\|_{C^{1,1}} \right) \left\| f(s) - \hat{f}(s) \right\|_{C^1} + D^2 B_{df}^{\infty - 1} \sum_{k=1}^{D} \sum_{j=1}^{D} \left| \frac{\partial f_j}{\partial s_k}(s) - \frac{\partial \hat{f}_j}{\partial s_k}(s) \right| \\
\leq \left\| \frac{df^{-1} \circ f}{ds}(s) - \frac{df^{-1} \circ \hat{f}}{ds}(s) \right\|_{op}^{d} \\
\leq (D^2 + D)^{d-1} \left\{ \sum_{j=1}^{D} \left( D^{3/2} B_{df}^{\infty} \left( \sum_{k=1}^{D} \left\| f_k^{-1} \right\|_{C^{1,1}} \right) \left| f_j(s) - \hat{f}_j(s) \right| \right)^d + \sum_{k=1}^{D} \sum_{j=1}^{D} \left( D^{3/2} B_{df}^{\infty - 1} \left| \frac{\partial f_j}{\partial s_k}(s) - \frac{\partial \hat{f}_j}{\partial s_k}(s) \right| \right)^d \right\} \\
where we used \((\sum_{i=1}^{L} a_i)^d \leq L^{d-1} (\sum_{i=1}^{L} a_i^d)\) for \(a_i \geq 0\), which follows from Hölder inequality. Hence,

\[
\int \left\| \frac{df^{-1} \circ f}{ds} (s) - \frac{df^{-1} \circ \hat{f}}{ds} (s) \right\|_\text{op}^d \, ds
\]

\[
\leq D^{2d-1}(D + 1)^{d-1} \left[ \left( B_{\partial f}^\infty \sum_{k=1}^{D} \| f_k^{-1} \|_{C^{1,1}} \right) \sum_{j=1}^{D} \int \| f_j (s) - \hat{f}_j (s) \|^d \, ds
\]

\[
+ (B_{\partial f^{-1}}^\infty)^d \sum_{k=1}^{D} \left( \sum_{j=1}^{D} \int \left\| \frac{\partial f_j}{\partial s_k} (s) - \frac{\partial \hat{f}_j}{\partial s_k} (s) \right\|^d \, ds \right) \right]
\]

\[
\leq (D + 1)^{2d-2} \left( (B_{\partial f}^\infty)^d \left( \sum_{k=1}^{D} \| f_k^{-1} \|_{C^{1,1}} \right) \sum_{j=1}^{D} \| f_j - \hat{f}_j \|_{W^{1,d}}^d + (B_{\partial f^{-1}}^\infty)^d \sum_{j=1}^{D} \| f_j - \hat{f}_j \|_{W^{1,d}}^d \right)
\]

\[
\leq C_d \sum_{j=1}^{D} \| f_j - \hat{f}_j \|_{W^{1,d}}^d .
\]

Therefore,

\[
\int \left| 1 - (Jf^{-1} \circ \hat{f}) (s) \right| \, ds
\]

\[
\leq \sum_{d=1}^{D} \binom{D}{d} \int \left\| \frac{df^{-1} \circ f}{ds} (s) - \frac{df^{-1} \circ \hat{f}}{ds} (s) \right\|_\text{op}^d \, ds
\]

\[
\leq DC_1 \sum_{j=1}^{D} \| f_j - \hat{f}_j \|_{W^{1,1}} + \sum_{d=2}^{D} \binom{D}{d} \sum_{j=1}^{D} \| f_j - \hat{f}_j \|_{W^{1,d}}^d \frac{\kappa_2(f - \hat{f})}{\kappa_2(f - \hat{f})}
\]

\[
\square
\]

Lemma 11 used the following lemma to bound the difference in Jacobian determinants.

**Lemma 12** (Determinant perturbation bound \cite{IpsenRehman2008} Corollary 2.11). Let \(A\) and \(E\) be \(D \times D\) complex matrices. Then,

\[
| \det(A) - \det(A + E) | \leq \sum_{d=1}^{D} \binom{D}{d} \| A \|_{\text{op}}^{D-d} \| E \|_{\text{op}}^d .
\]

### C.8 Comparison of Rademacher complexities

The following consideration demonstrates how the effective complexity measure \(\mathcal{R}\) in Theorem 3 resulting from the proposed method may enjoy a relaxed dependence on the input dimensionality compared to the ordinary empirical risk minimization. To do so, we first recall the definition of the ordinary Rademacher complexity and a standard performance guarantee derived based on it.

**Definition 2** (Ordinary Rademacher complexity). The ordinary empirical risk minimization finds the candidate hypothesis by

\[
\hat{g} \in \arg \min_{g \in \mathcal{G}} \hat{R}(g),
\]

where

\[
\hat{R}(g) := \frac{1}{n} \sum_{i=1}^{n} \ell(g, Z_i) = \frac{1}{n} \sum_{i=1}^{n} \ell(g, \hat{f}(S^{(1)}_i, \ldots, S^{(D)}_i))
\]
and the corresponding ordinary Rademacher complexity $\mathcal{R}_{\text{ord}}(\mathcal{G})$ is

$$\mathcal{R}_{\text{ord}}(\mathcal{G}) := \frac{1}{n} \mathbb{E}_G \mathbb{E}_\sigma \left[ \sup_{g \in \mathcal{G}} \sum_{i=1}^n \sigma_i \ell(S_i^{(1)}, \ldots, S_i^{(D)}) \right]$$

where $\{\sigma_i\}_{i=1}^n$ are independent uniform sign variables and we denoted $\ell(s^{(1)}, \ldots, s^{(D)}) = \ell(g, \hat{f}(s^{(1)}, \ldots, s^{(D)}))$ by abuse of notation. This yields the standard Rademacher complexity based bound. Applying Lemma 5 and using the same proof technique, we have that with probability at least $1 - \delta$,

$$R(\hat{g}) - R(g^*) \leq 2 \sup_{g \in \mathcal{G}} |R(g) - \hat{R}(g)| \leq 4\mathcal{R}_{\text{ord}}(\mathcal{G}) + 2B \sqrt{\frac{\log(2/\delta)}{2n}}.$$

Therefore, we make a comparison of these two complexity measures by taking an example. To recall, the effective Rademacher complexity can be written as,

$$\mathcal{R}_{\text{eff}} = \mathcal{R}(g, \hat{f}) = \mathcal{R}(g, \hat{f}) + \frac{1}{n} \mathbb{E}_G \mathbb{E}_\sigma \left[ \sup_{g \in \mathcal{G}} \sum_{i=1}^n \sigma_i \ell(S_i^{(1)}, \ldots, S_i^{(D)}) \right].$$

\textbf{Remark 3 (Comparison of Rademacher complexities).} As an example, consider $\mathcal{H}$, the set of $L$-Lipschitz functions (with respect to infinity norm) on the unit cube $[0, 1]^d$. It is well-known that there exists a constant $C > 0$ such that the following holds (Wainwright, 2019, Example 5.10, p.129) for sufficiently small $t > 0$:

$$\log N(t, \mathcal{H}, \|\cdot\|_\infty) \asymp (C/t)^d. \tag{9}$$

Here, $a(t) \asymp b(t)$ indicates that there exist $k_1, k_2 > 0$ such that, for sufficiently small $t$, it holds that $k_1 b(t) \leq a(t) \leq k_2 b(t)$. On the other hand, the well-known discretization argument implies that there exist constants $c$ and $B$ such that for any $t \in (0, B]$, the following relation between the Rademacher complexity and the metric entropy holds:

$$\mathcal{R}_{\text{ord}}(\mathcal{H}) \leq t + c \sqrt{\frac{\log N(t, \mathcal{H}, \|\cdot\|_\infty)}{n}}. \tag{10}$$

Substituting Eq. (9) into Eq. (10), we can find that, for large enough $n$, the right hand side is minimized at $t = (c \cdot C^2 \cdot \frac{d}{2})^{\frac{1}{2d}} \cdot n^{-\frac{1}{2d}}$. This yields

$$\mathcal{R}_{\text{ord}}(\mathcal{H}) \leq \tilde{C} \cdot n^{-\frac{1}{2d}} \tag{11}$$

with a new constant $\tilde{C} = (c \cdot C^2 \cdot \frac{d}{2})^{\frac{1}{2d}} + c \cdot C^2 \cdot \left( c \cdot C^2 \cdot \frac{d}{2} \right)^{-\frac{1}{2d}}$. Therefore, by substituting $d = D$ in Eq. (11), the metric-entropy based bound on the ordinary Rademacher complexity exhibits exponential dependence on the input dimension as

$$\mathcal{R}_{\text{ord}}(\mathcal{H}) \leq O \left( n^{-\frac{1}{2D}} \right),$$

which is a manifestation of the curse of dimensionality. On the other hand, by following a similar calculation, we can see that the effective Rademacher complexity $\mathcal{R}_{\text{eff}}(\mathcal{G})$ avoids an exponential dependence on the input dimension $D$. By substituting $d = 1$ in Eq. (11), we can see

$$D\mathcal{R}_{\text{eff}}(\mathcal{G}) \leq \mathcal{R}_{\text{ord}}(\mathcal{H}_1) + \cdots + \mathcal{R}_{\text{ord}}(\mathcal{H}_D) \leq O \left( n^{-\frac{1}{2}} \right),$$

where $\mathcal{H}_j := \{E_{S^{(1)}_1, \ldots, S^{(D)}_D} h(S^{(1)}_1, \ldots, S^{(j-1)}_{j-1}, S^{(j)}_{j-1}^{(j-1)}, \cdots, S^{(j)}_{j-1}^{(j+1)}, \ldots, S^{(D)}_D) : h \in \mathcal{H} \}$. This is because the Lipschitz constant of functions in $\mathcal{H}_j$ is at most $L$ (i.e., the Lipschitz constant does not increase by the marginalization procedure) because for any $h \in \mathcal{H}_j$,

$$|h(x) - h(y)|$$

$$= \left| E_{S^{(1)}_1, \ldots, S^{(D)}_D} [h(S^{(1)}_1, \ldots, S^{(j-1)}_{j-1}, x, S^{(j)}_{j-1}^{(j+1)}, \ldots, S^{(D)}_D) - h(S^{(1)}_1, \ldots, S^{(j-1)}_{j-1}, y, S^{(j+1)}_{j-1}, \ldots, S^{(D)}_D)] \right|$$

$$\leq E_{S^{(1)}_1, \ldots, S^{(D)}_D} \| (S^{(1)}_1, \ldots, S^{(j-1)}_{j-1}^{(j-1)}, x, S^{(j)}_{j-1}^{(j+1)}, \ldots, S^{(D)}_D) - (S^{(1)}_1, \ldots, S^{(j-1)}_{j-1}^{(j-1)}, y, S^{(j+1)}_{j-1}^{(j+1)}, \ldots, S^{(D)}_D) \|$$

$$= E_{S^{(1)}_1, \ldots, S^{(D)}_D} \| (0, \ldots, 0, x - y, 0, \ldots, 0) \|$$

$$= L \cdot |x - y|. \tag{12}$$
C.9 Remark on higher order Sobolev norms

Here, we comment on how the term $\kappa_2(f - \hat{f})$ is treated as a higher order term of $f - \hat{f}$.

**Remark 4** (Higher order Sobolev norms). Let us assume that $\text{supp} \, q \cup \text{supp} \, \hat{q}$ is contained in a compact set $\tilde{S}$ for all $f$ considered. Note that for $d \in [D]$,

$$\int_{\tilde{S}} |h(s)|^d ds \leq (V_{\tilde{S}})^{d/D} \left( \int_{\tilde{S}} |h(s)|^D ds \right)^{d/D}$$

by Hölder’s inequality, where we defined $V_{\tilde{S}} := \int_{\tilde{S}} 1 ds$, hence we have $\| \cdot \|_{L^d(\tilde{S})} \leq (V_{\tilde{S}})^{1/d} \| \cdot \|_{L^D(\tilde{S})}$. By applying the relation to each term in the definition of $\| \cdot \|_{W^{1,d}}$, we obtain

$$\|f\|_{W^{1,d}} \leq (V_{\tilde{S}})^{1/d} \|f\|_{W^{1,D}}$$

Thus we obtain

$$\kappa_2(f - \hat{f}) = \sum_{d=2}^{D} \binom{D}{d} C_d \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,d}}$$

$$\leq \sum_{d=2}^{D} \binom{D}{d} (V_{\tilde{S}})^{1/d} C_d \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,d}}$$

$$\leq O \left( \sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,D}}^2 \right) \quad (\hat{f} \to f).$$

By also replacing $\sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,1}}$ with $\sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,D}}$ in Theorem 3, we can see more clearly that $\kappa_2(f - \hat{f})$ is a higher order term of $\sum_{j=1}^{D} \|f_j - \hat{f}_j\|_{W^{1,D}}$.

D Details and Proofs of Theorem 1

Here, we provide the proof of Theorem 1. We reuse the notation and terminology from Section C of this Supplementary Material. We prove the uniformly minimum variance property of the proposed risk estimator under the ideal situation of $\hat{f} = f$.

**Theorem 4** (Known causal mechanism case). Assume $\hat{f} = f$. Then, for all $g \in G$, we have that $\hat{R}(g)$ is the uniformly minimum variance unbiased estimator of $R(g)$. As a special case, it has a smaller variance than the ordinary empirical risk estimator: $\forall q \in Q, \forall g \in G, \text{Var}(\hat{R}(g)) \leq \text{Var}(\hat{R}(g))$.

**Proof.** The proof is a result of the following two facts. When $\hat{q} \in Q$, the estimator $\hat{R}(g)$ becomes the generalized U-statistic of the statistical functional Eq. (6). Furthermore, when $\hat{f} = f$, Eq. (6) coincides with $R(g)$ because the approximation error is zero. Since we assume $\hat{f} = f$ we have $\hat{q} = q \in Q$ and hence both of the statements above hold. Therefore, by Lemma 13 the first assertion of the theorem follows. The last assertion of the theorem follows as a special case as $\hat{R}(g)$ is an unbiased estimator of $R(g)$ for $q \in Q$. 
From here, we confirm the above statements by calculation. We first show that \( \hat{R}(g) \) is the generalized U-statistic. To see this, observe that the statistical functional Eq. (6) allows the following expression given \( q \in Q \):

\[
\int \ell(s_1, \ldots, s_D) \tilde{q}(s_1) \cdots \tilde{q}(s_D) ds_1 \cdots ds_D
\]

\[
= \int \sum_{\pi \in \Theta_D} \ell(g, \hat{f}(s_{x(1)}^{(1)}, \ldots, s_{x(D)}^{(D)})) \tilde{q}(s_1) \cdots \tilde{q}(s_D) ds_1 \cdots ds_D
\]

\[
= \int \sum_{\pi \in \Theta_D} \ell(g, \hat{f}(s_{x(1)}^{(1)}, \ldots, s_{x(D)}^{(D)})) \prod_d \tilde{q}^{(d)}(s_d^{(1)}) \cdots \prod_d \tilde{q}^{(d)}(s_D^{(d)}) ds_1 \cdots ds_D
\]

\[
= \int \sum_{\pi \in \Theta_D} \ell(g, \hat{f}(s^{(1)}, \ldots, s^{(D)})) \tilde{q}_1(s^{(1)}) \cdots \tilde{q}_D(s^{(D)}) ds^{(1)} \cdots ds^{(D)}.
\]

This is a regular statistical functional of degrees \((1, \ldots, 1)\) with the kernel \( \ell(g, \hat{f}(s^{(1)}, \ldots, s^{(D)})) \). On the other hand, we have

\[
\hat{R}(g) = \frac{1}{n^D} \sum_{(i_1, \ldots, i_D) \in [n]^D} \ell(S_{i_1}, \ldots, S_{i_D}) = \frac{1}{n^D} \sum_{(i_1, \ldots, i_D) \in [n]^D} \ell(g, \hat{f}(S_{i_1}^{(1)}, \ldots, S_{i_D}^{(D)}))
\]

because the summations run through all combinations with replacement. This combined with the fact that \( \{S_{i}^{(d)}\}_{i,d} \) are jointly independent when \( q \in Q \) yields that \( \hat{R}(g) \) is the generalized U-statistic for Eq. (6).

Now we show that Eq. (6) coincides \( R(g) \). Given \( \hat{f} = f \), we have

\[
R(g) = \int q(s) \ell(g, f(s)) ds
\]

\[
= \int q(s) \ell(g, \hat{f}(s)) ds \quad \text{(By } f = \hat{f})
\]

\[
= \int q_1(s^{(1)}) \cdots q_D(s^{(D)}) \ell(g, \hat{f}(s^{(1)}, \ldots, s^{(D)})) ds^{(1)} \cdots ds^{(D)} \quad \text{(by } q \in Q)
\]

\[
= \int \tilde{q}_1(s^{(1)}) \cdots \tilde{q}_D(s^{(D)}) \ell(g, \hat{f}(s^{(1)}, \ldots, s^{(D)})) ds^{(1)} \cdots ds^{(D)} \quad \text{(by } q = \tilde{q})
\]

\[
= \int \tilde{q}(s_1, \ldots, s_D) \tilde{q}(s_1) \cdots \tilde{q}(s_D) ds_1 \cdots ds_D. \quad (\because \text{symmetry})
\]

The following well-known lemma states that a generalized U-statistic is a uniformly minimum variance unbiased estimator.

**Lemma 13** (Uniformly minimum variance property of a generalized U-statistic). Let \( \theta : Q \to \mathbb{R} \) be a regular statistical functional with kernel \( \psi : \mathbb{R}^{k_1} \times \cdots \times \mathbb{R}^{k_L} \to \mathbb{R} \) (Clémençon et al., 2016), i.e.,

\[
\theta(q) = \int \psi((x_1^{(1)}, \ldots, x_{k_1}^{(1)}), \ldots, (x_1^{(L)}, \ldots, x_{k_L}^{(L)})) \prod_{j=1}^{k_1} q_1(x_j^{(1)}) dx_j^{(1)} \cdots \prod_{j=1}^{k_L} q_L(x_j^{(L)}) dx_j^{(L)}.
\]

Given samples \( \{x_i^{(l)}\}_{i=1}^{n_l} \overset{i.i.d.}{\sim} q_l(n_l \geq k_l \text{ and } l = 1, \ldots, L) \), let \( \mathrm{GU}_{(n_1, \ldots, n_L)}(\psi) \) be the corresponding generalized U-statistic

\[
\mathrm{GU}_{(n_1, \ldots, n_L)}(\psi) := \frac{1}{\prod (n_l)^{k_l}} \sum \psi \left( \left( x_1^{(1)}, \ldots, x_{k_1}^{(1)} \right), \ldots, \left( x_1^{(L)}, \ldots, x_{k_L}^{(L)} \right) \right).
\]

where \( \sum \) denotes that the indices run through all possible combinations (without replacement) of the indices. Then, \( \mathrm{GU}_{(n_1, \ldots, n_L)}(\psi) \) is the uniformly minimum variance unbiased estimator of \( \theta \) on \( Q \).

**Proof.** The assertion can be proved in a parallel manner as the proof of (Lee, 1990, Section 1.1, Lemma B)
Remark 5 (Relation to the UMVUE property of $\hat{R}(g)$). The result in Theorem 4 is not contradictory to the fact that the sample average $\bar{R}(g)$ is a U-statistic of degree-1 and hence the minimum variance among all unbiased estimator of $R(g)$ on $P$, where $P$ is a set of distributions containing all absolutely continuous distributions (Lee, 1990). Specifically, $\bar{R}(g)$ is not generally an unbiased estimator of $R(g)$ on $P \setminus Q$, even if $\hat{f} = f$. While $\bar{R}(g)$ satisfies the D-sample symmetry condition, the same does not hold for $\hat{R}(g)$. By restricting the attention to $Q$, the estimator $\hat{R}(g)$ achieves a smaller variance than $\bar{R}(g)$. 
