Characterizing the Fundamental Trade-offs in Learning Invariant Representations

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Abstract

Many applications of representation learning, such as privacy-preservation, algorithmic fairness and domain adaptation, desire explicit control over semantic information being discarded. This goal is formulated as satisfying two objectives: maximizing utility for predicting a target attribute while simultaneously being independent or invariant with respect to a known semantic attribute. Solutions to such problems lead to trade-offs between the two objectives when they are competing with each other. While existing works study bounds on these trade-offs, three questions still remain outstanding: What are the exact fundamental trade-offs between utility and invariance?, 2) What is the optimal dimensionality of the representation?, and 3) What are the encoders (mapping data to a representation) that achieve the exact fundamental trade-offs and how can we estimate them from data? This paper addresses these questions. We adopt a functional analysis perspective and derive closed-form solutions for the global optima of the underlying optimization problems under mild assumptions, which in turn yields closed formulae for the exact trade-offs, optimal representation dimensionality and the corresponding encoders. We also numerically quantify the trade-offs on representative problems and compare them to those achieved by baseline invariant representation learning algorithms.
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Figure 1: Invariant representation learning (IRL) seeks a representation $Z$ that contains enough information for downstream target predictor $g_Y$ while being independent of the semantic attribute $S$. We characterize two IRL fundamental trade-offs exactly, (a) label-space trade-off induced by an ideal representation $Z_I$, and (b) data-space trade-off induced by a learned representation $Z_D$.

1 Introduction

Real-world applications of representation learning often has to contend with objectives beyond predictive performance. These include cost functions pertaining to, invariance (e.g., to photometric or geometric variations), semantic independence (e.g., w.r.t to age or race for face recognition systems), privacy (e.g., mitigating leakage of sensitive information [1]), algorithmic fairness (e.g., demographic parity [2]), and generalization across multiple domains [3], to name a few.

At its core, the goal of the aforementioned formulations of representation learning is to satisfy two competing objectives, extracting as much information necessary to predict a target label $Y$ (e.g., face identity) while intentionally and permanently suppressing information about a desired semantic attribute $S$ (e.g., age or gender). Let $Z$ be a representation from which the target attribute $Y$ can be predicted. When $Y$ and $S$ are considerably dependent, then learning a representation $Z$ that is invariant w.r.t. the semantic attribute $S$ (i.e., ensuring $Z \perp S$) will necessarily degrade the performance of the target prediction task i.e., there exists a trade-off between utility and semantic independence.

The existence of a trade-off has been well established, both theoretically and empirically, under various contexts of representation learning such as fairness [4, 5, 6, 7], invariance [8], and domain adaptation [9]. However, a majority of this body of work only establishes bounds on the trade-off, as opposed to precise characterization. As such a number of aspects of the trade-off in invariant representation learning (IRL) are unknown, including, i) exact characterization of the fundamental trade-off inherent to IRL, ii) the minimal dimensionality of the representation $Z$ necessary to achieve a desired optimal trade-off point, and iii) a learning algorithm that achieves the exact fundamental trade-off.

This paper establishes the aforementioned characteristics for the trade-offs in IRL that arise from two fundamentally different scenarios as shown in Fig. 1.

1. **Label-Space Trade-off (LST)** shown in Fig. 1a is induced purely by the statistical dependency between $Y$ and $S$. In this case the *ideal* representation $Z_I$ is unconstrained by input data $X$ and can be any random vector (RV) in the space of finite variance RVs.

2. **Data-Space Trade-off (DST)** shown in Fig. 1b is induced by the statistical dependency between $Y$ and $S$ conditioned on the input data $X$. The representation $Z_D = f(X)$ is now a function of input data $X$ where the encoder $f(\cdot)$ is a Borel-measurable function.

Before formally defining these trade-offs (see Fig. 2 for an illustration), we describe how they are qualitatively different. Consider an example where $Y \perp S$, $X = Y + S$ and the target task is to regress $Y$ from $X$ through representation $Z$ with mean-squared error (MSE) loss. In the LST scenario, one can learn a

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1 Under different scenarios such as $Y$ and $S$ being discrete, continuous or combinations thereof.
Figure 2: We consider two fundamental trade-offs between utility (i.e., performance of target predictor) and dependence measure \( \text{dep}(Z, S) \) by an optimal learner in the hypothesis class of Borel-measurable functions. Trade-off \( L \) (LST) is induced by the joint distribution of the labels \( p_{YS} \). Trade-off \( D \) (DST) is induced by the joint distribution of the labels conditioned on features \( p_{YS|X} \). Trade-off \( F \) is a relaxed version of DST obtained by either using a surrogate measure of dependence, e.g., adversarial learning \([\text{3}]\) or from a constrained hypothesis class \([\text{10}]\), or from using sub-optimal optimization algorithms.

representation that is independent of \( S \) with no loss in target performance simply by choosing \( Z_L = Y \), i.e., there is no trade-off between utility and invariance. In the DST scenario the Bayes optimal prediction \( \hat{Y} = X - \mathbb{E}_S[S] \) is dependent on \( S \) since \( X \) is dependent on \( S \). Therefore, the corresponding optimal representation \( Z_D = f_{\text{opt}}(X) \) is a function of \( S \) and cannot be independent of it i.e., there exists a trade-off between utility and invariance.

**Definition 1. Label Space Trade-Off (LST)** When the target hypothesis class, \( \mathcal{H}_Y \) contains all Borel-measurable functions, this trade-off can be defined as:

\[
\inf_{Z \in L^2} \left\{ (1 - \tau) \inf_{g_Y \in \mathcal{H}_Y} \mathbb{E}_{X,Y} \left[ \mathcal{L}_Y \left( g_Y(Z) , Y \right) \right] + \tau \text{dep}(Z, S) \right\}
\]

(1)

where \( \mathcal{L}_Y(\cdot, \cdot) \) is the loss for predicting the attribute \( Y \) and \( L^2 \) is the space of all RVs with finite variance (i.e., \( \mathbb{E}_Z \left[ ||Z - \mathbb{E}_Z[Z]||^2 \right] < \infty \)). The function \( \text{dep}(\cdot, \cdot) \geq 0 \) is a parametric or non-parametric measure of statistical dependence i.e., \( \text{dep}(Q, U) = 0 \) implies \( Q \) and \( U \) are independent, and \( \text{dep}(Q, U) > 0 \) implies \( Q \) and \( U \) are dependent with larger values indicating greater degrees of dependence. The scalar \( \tau \in [0, 1) \) is a user defined parameter that controls the trade-off between the two objectives, with \( \tau = 0 \) being the standard scenario that has no independence constraints w.r.t \( S \), while \( \tau \rightarrow 1 \) enforces \( Z \perp \!\!\!\perp S \).

This definition corresponds to the optimal trade-off \( L \) in Figure 2 and is obtained by an ideal representation \( Z_L \) that is not constrained by the input data \( X \). For example, if \( \tau = 0 \), the ideal representation \( Z_L \) is perfectly aligned with the target label \( Y \). This means that if \( Z = Y \) and \( g_Y \) is the identity function, perfect prediction of the target attribute is feasible. However, there might not exist any encoder-predictor pair such that \( Y = g_Y(f(X)) \) if \( X \) does not contain sufficient information about \( Y \). Therefore, this trade-off corresponds to the best trade-off that any combination of data \( X \) and learnable encoder \( f \) can aspire to.
**Definition 2. Data Space Trade-Off (DST)** When the hypothesis classes, $\mathcal{H}_X, \mathcal{H}_Y$ contain all Borel-measurable functions, this trade-off can be defined as:

$$\inf_{f \in \mathcal{H}_X} \left\{ (1 - \tau) \inf_{g_Y \in \mathcal{H}_Y} \mathbb{E}_{X,Y} \left[ \mathcal{L}_Y \left( g_Y (f(X)), Y \right) \right] + \tau \text{dep}(f(X), S) \right\}$$

where $f$ is the encoder that extracts representation $Z$ from $X$ and $g_Y$ predicts $\hat{Y}$ from the representation $Z$.

Including all measurable functions in $\mathcal{H}_X$ and $\mathcal{H}_Y$ ensures that the best possible trade-off is included within the feasible solution space. For example, when $\tau = 0$ and $\mathcal{L}_Y(\cdot, \cdot)$ is MSE, the optimal Bayes estimation $g_Y(f(X)) = \mathbb{E}_Y [Y | X]$ is reachable. This definition corresponds to the trade-off $D$ in Figure 2 and it is necessarily dominated by (or equal to) the LST.

**Contributions:** i) We design a dependence measure that accounts for all modes of dependence between $Z$ and $S$ while allowing for analytical tractability. ii) We adopt a functional analysis perspective and obtain closed-form solutions for the IRL optimization problems under mild assumptions. Consequently, we characterize the Label-Space Trade-off and Data-Space Trade-off exactly. iii) We obtain a (scalable) closed-form estimator for the encoder that achieves the optimal trade-offs and establish its consistency. iv) We numerically quantify the fundamental trade-offs on an illustrative problem as well as large scale real-world datasets, Folktables [11] and CelebA [12], and compare them to those obtained by existing solutions.

## 2 Related Work

### 2.1 Semantically Independent Representations

The basic idea of representation learning that discards unwanted semantic information has been explored under many contexts like invariant, fair, or privacy-preserving learning. In domain adaptation [13][14][15], the goal is to learn features that are independent of the data domain. In fair learning [16][17][18][19][20][21][22][23][24][25][26][27][28][29][30][10], the goal is to discard the demographic information that leads to unfair outcomes. Similarly, there is growing interest in mitigating unintended leakage of private information from representations [31][32][1][33][34].

A vast majority of this body of work is empirical in nature. They implicitly look for a single or multiple points on the trade-off between utility and semantic information and do not explicitly seek to characterize the whole trade-off front. Overall, these approaches are not concerned with or aware of the inherent fundamental utility-invariance trade-offs. In contrast, this paper seeks to exactly characterize these trade-offs, and proposes practical learning algorithms that achieves these trade-offs.

### 2.2 Adversarial Representation Learning

Most practical approaches for learning fair, invariant, domain adaptive or privacy-preserving representations discussed above are based on adversarial representation learning (ARL). ARL is typically formulated as,

$$\inf_{f \in \mathcal{H}_X} \left\{ (1 - \tau) \inf_{g_Y \in \mathcal{H}_Y} \mathbb{E}_{X,Y} \left[ \mathcal{L}_Y \left( g_Y (f(X)), Y \right) \right] - \tau \inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X,S} \left[ \mathcal{L}_S \left( g_S (f(X)), S \right) \right] \right\},$$

where $\mathcal{L}_S(\cdot, \cdot)$ is the loss function of a hypothetical adversary $g_S$ who intends to extract the semantic attribute $S$ through the best predictor within the hypothesis class $\mathcal{H}_S$. ARL is a special case of the Data Space Trade-Off in (2) where the negative loss of the adversary, $- \inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X,S} \left[ \mathcal{L}_S \left( g_S (f(X)), S \right) \right]$ plays the role of $\text{dep}(f(X), S)$. However, this form of adversarial learning suffers from a drawback. The induced measure does not account for all modes of non-linear dependence between $S$ and $Z$ if the loss function $\mathcal{L}_S$ is MSE or...
cross-entropy \[35, 36\] (see Appendix I for a formal proof). This implies that an optimal adversary may not necessarily lead to a representation \(Z\) that is statistically independent of \(S\). Therefore, the adversary loss in ARL should be carefully designed \[7\] to account for all modes of dependence between \(Z\) and \(S\).

### 2.3 Trade-Offs in Invariant Representation Learning:

Prior work has established the existence of trade-offs in invariant representation learning, both empirically and theoretically. We categorize them based on properties of interest.

**Restricted Class of Attributes:** Majority of existing work considers IRL trade-offs under restricted settings, i.e., binary and/or categorical attributes \(Y\) and \(S\). For instance, \[5\] uses information theoretic tools and characterizes the utility-fairness trade-off in terms of lower bounds when both \(Y\) and \(S\) are binary labels. Later \[37\] provided both upper and lower bound for the binary labels. By leveraging Chernoff bound, \[38\] proposed a construction method to generate an ideal representation beyond input data to achieve perfect fairness while maintaining the best performance on target task for equalized odds. In the case of categorical features, a lower bound on utility-fairness trade-off has been provided by \[39\]. In contrast to this body of work, our trade-off analysis applies to multi-dimensional discrete and/or continuous attributes where we find the exact optimal trade-offs. To the best of our knowledge, the only prior works with a more general setting where \(Y\) and \(S\) can be continuous are \[10\] and \[8\]. However, in \[8\], both \(S\) and \(Y\) are restricted to be continuous or discrete at the same time (e.g., it is not possible to have \(Y\) continuous while \(S\) is discrete).

**Dependence Measure:** A majority of existing work considers adversarial losses optimizing MSE or cross-entropy loss as a surrogate measure of dependence between the representation \(Z\) and the semantic attribute \(S\). However, such a measure cannot capture all modes of statistical dependency if \(S\) is not binary (see \[35\] and Appendix I for more details). Some examples deploying MSE based adversarial loss are \[39, 8, 10\]. For discrete \(S\) \[8\] employ mutual information (MI) as a dependence measure to solutions at the end points of the trade-off i.e., \(\tau \rightarrow 0\) and \(\tau \rightarrow 1\). However, estimating MI between multi-dimensional continuous \(Z\) and \(S\) is computationally challenging. For continuous \(S\), \[7\] employs Wasserstein distance \[40\] between \(g_S(Z)\) and \(S\) as the adversarial loss, which potentially accounts for all modes of dependence between \(Z\) and \(S\). In contrast, we employ a dependence measure that is both computationally tractable for multi-dimensional continuous/discrete RVs and capable of capturing all modes of dependency through a universal RKHSs.

**Characterizing Exact vs Bounds on Trade-Off:** To the best of our knowledge, all existing approaches except \[10\], which obtains the trade-off for the mean dependence measure induced by an adversary optimizing MSE loss, characterize the trade-off in terms of upper and/or lower bounds. In contrast, we *exactly* characterize both data and label space trade-offs with exact closed-form expressions for a full measure of dependence.

**Optimal Encoder and Representation:** Apart from the *exact* fundamental trade-offs another quantity of practical interest is the optimal encoder that achieves the fundamental trade-offs and its corresponding representation. Existing work which only study bounds on the trade-offs do not obtain the encoder that achieves those bounds. \[10\] do develop a representation learning algorithm that obtains the globally optimal encoder and representation but only under a linear dependence measure between \(Z\) and \(S\) induced by an MSE adversarial loss. In contrast, we obtain a closed for solution for the optimal encoder and its corresponding representation while considering all non-linear dependencies between \(Z\) and \(S\).

### 3 Problem Setting

We first introduce the mathematical notations used in this paper and describe the invariant representation learning setup.

**Notations:** Scalars are denoted by regular lower case letters, e.g. \(r, \tau\). Deterministic vectors are denoted by boldface lower case letters, e.g. \(x, s\). We denote both scalar-valued and multi-dimensional RVs by regular
We assume that the encoder consists of an r-dimensional encoder $f(\cdot)$ belonging to RKHS $\mathcal{H}_X$. ii) A measure of dependence that accounts for all linear and non-linear dependencies between the representation $Z$ and semantic attribute $S$ via the covariance between $f(X)$ and $\beta_S(S)$ where $X$ is the input data and $\beta_S(\cdot)$ belongs to a RKHS $\mathcal{H}_S$. iii) A measure of dependency between $f(X)$ and the target attribute $Y$ defined similar to the one for $S$.

**Problem Setup:** Consider the probability space $(\Omega, \mathcal{F}, \mathbb{P})$, where $\Omega$ is the sample space, $\mathcal{F}$ is a $\sigma$–algebra on $\Omega$, and $\mathbb{P}$ is a probability measure on $\mathcal{F}$. We assume that the joint RV $(X, Y, S)$, containing the input data $X \in \mathbb{R}^{d_x}$, the target label $Y \in \mathbb{R}^{d_y}$ and the semantic attribute $S \in \mathbb{R}^{d_s}$, is a random vector on $(\Omega, \mathcal{F})$ with joint distribution $p_{X,Y,S}$. Furthermore, $Y$ and $S$ can also belong to any finite set like a categorical set. This setting, enables us to work with both classification and multi-dimensional regression target tasks where the semantic attribute can be either discrete, categorical or multi-dimensional continuous.

**Assumption 1.** We assume that the encoder consists of $r$ functions from $\mathbb{R}^{d_x}$ to $\mathbb{R}$ in a universal RKHS $(\mathcal{H}_X, k_X(\cdot, \cdot))$ (e.g., RBF kernel), where universality ensures that $\mathcal{H}_X$ can approximate any Borel-measurable function with arbitrary precision [41].

Now, the representation vector $Z$ can be expressed as

$$Z = f(X) := \left[ f_1(X), \cdots, f_r(X) \right]^T \in \mathbb{R}^r, \quad f_j(\cdot) \in \mathcal{H}_X \forall j = 1, \ldots, r,$$

(4)

where $r$ is the dimensionality of the representation $Z$. As discussed in Corollary 4.1 unlike common practice where $r$ is chosen arbitrarily, it is an object of interest for optimization. We consider a general scenario where both $Y$ and $S$ can be continuous or discrete, or one of $Y$ or $S$ is continuous while the other is discrete. To do this, we substitute the target loss, $\inf_{g_Y} \mathbb{E}_{X,Y} \mathcal{L}_Y(g_Y(Z), Y)$ in (2) with the negative of a non-parametric measure of dependence i.e., $-\text{dep}(Z, Y)$. Such a substitution is justifiable as follows.

Maximizing statistical dependency between the representation $Z$ and the target attribute $Y$ can flexibly learn a representation that is effective for different downstream target tasks, including, regression, classification, clustering, etc [42]. Particularly, Theorem 6 of Section H in the appendix shows that with an appropriate choice of $\text{dep}(Z, Y)$, we can learn a representation that lends itself to a predictor that performs as well as the Bayes prediction $\mathbb{E}_X[Y|X]$. Furthermore, in unsupervised settings, where there is no target attribute $Y$, the target loss can be replaced with $\text{dep}(Z, X)$, which implicitly forces the representation $Z$ to be as dependent on the input data $X$. This scenario is of practical interest when a data producer aims to provide a representation that is independent of a desired semantic attribute for any arbitrary downstream target task.
4 Choice of Dependence Measure

We start by designing $\text{dep}(Z, S)$, and $\text{dep}(Z, Y)$ follows similarly. Accounting for all possible non-linear dependence relations between the random variables (or vectors) is a key desiderata of dependence measures. Examples of such measures include information theoretic measures such as MI (e.g., MINE \[43\]). However, calculating MI for multi-dimensional continuous representation is analytically challenging and computationally intractable. Kernel measures (e.g., HSIC \[44\]) are an alternative solution with the attractive properties of being computationally feasible/efficient and analytically tractable \[45\]. Therefore, we adopt a kernel based method as our choice of dependence measure.

Principally, $Z$ and $S$ are independent iff $\text{Cov}(\alpha(Z), \beta_S(S))$ is zero for all $\alpha(\cdot) : \mathbb{R}^r \rightarrow \mathbb{R}$ and $\beta_S(\cdot) : \mathbb{R}^d_S \rightarrow \mathbb{R}$ belonging to some universal RKHSs \[45\]. The Hilbert-Schmidt Independence Criterion (HSIC) \[44\] is defined as,

$$\text{HSIC}(Z, S) := \sum_{\alpha \in \mathcal{U}_Z} \sum_{\beta_S \in \mathcal{U}_S} \text{Cov}^2(\alpha(Z), \beta_S(S)),$$

(5)

where a non-linear mapping is applied to both $Z$ and $S$, $\mathcal{U}_S$ is a countable orthonormal basis sets for $\mathcal{H}_S$, and $\mathcal{U}_Z$ is a countable orthonormal basis set for a given RKHS of functions from $\mathbb{R}^r$ to $\mathbb{R}$. However, since $Z = f(X)$ for $f(\cdot)$ in (4), evaluating $\text{Cov}(\alpha(Z), \beta_S(S))$ necessitates the application of a cascade of kernels which limits the analytical tractability of our solution. Therefore, we adopt a simplified version of HSIC that considers transformation on $S$ only but affords analytical tractability for solving the IRL optimization problem. This measure is defined as,

$$\text{dep}(Z, S) := \sum_{\beta_S \in \mathcal{U}_S} \sum_{j=1}^r \text{Cov}^2(f_j(X), \beta_S(S)),$$

(6)

The measure $\text{dep}(Z, S)$ still captures all modes of non-linear dependence under the assumption that the distribution of a low-dimensional projection of high-dimensional data is approximately normal \[46\], \[47\]. In other words, we assume that $(f(X), \beta_S(S))$ is approximately a jointly normal RV. In our numerical experiments in Section 6 we empirically observe that $\text{dep}(Z, S)$ enjoys a monotonic relation with HSIC, and captures all modes of dependency in practice, especially as $Z \perp \! \! \! \perp S$.

**Definition 3.** Let $D = \{(x_1, s_1, y_1), \ldots, (x_n, s_n, y_n)\}$ be the training data, containing $n$ i.i.d. samples of the joint distribution $p_{X, S, Y}$. Invoking the representer theorem \[48\], it follows that for each $f_j \in \mathcal{H}_X$ ($j = 1, \ldots, r$) we have $f_j(X) = \sum_{i=1}^n \theta_{ij} k_X(x_i, X)$ where $\theta_{ij}$’s are free scalars. Consequently, it holds that

$$f(X) = \Theta [k_X(x_1, X), \ldots, k_X(x_n, X)]^T,$$

where $\Theta \in \mathbb{R}^{r \times n}$ is a free parameter matrix.

**Lemma 1.** Let $K_X, K_S \in \mathbb{R}^{n \times n}$ be Gram matrices corresponding to $\mathcal{H}_X$ and $\mathcal{H}_S$, respectively, i.e. $(K_X)_{ij} = k_X(x_i, x_j)$ and $(K_S)_{ij} = k_S(s_i, s_j)$. Consider an empirical estimation of covariance as

$$\text{Cov}(f_j(X), \beta_S(S)) \approx \frac{1}{n} \sum_{i=1}^n f_j(x_i) \beta_S(s_i) - \frac{1}{n^2} \sum_{i=1}^n \sum_{k=1}^n f_j(x_i) \beta_S(s_k).$$

\[2\]We differ the proofs all Lemmas and Theorems to Appendices.
It follows that, an empirical estimation for \( \text{dep}(Z, S) \) is

\[
\text{dep}^{\text{emp}}(Z, S) := \frac{1}{n^2} \| \Theta K_X H L_S \|_F^2,
\]

where \( H = I_n - \frac{1}{n} 1_n 1_n^T \) is the centering matrix, and \( L_S \) is a full column-rank matrix in which \( L_S L_S^T = K_S \) (Cholesky factorization). The empirical estimator in (7) has a bias of \( O(n^{-1}) \) and a convergence rate of \( O(n^{-1/2}) \).

The dependence measure between \( Z \) and \( Y \) and its empirical version can be defined similarly.

5 Exact Fundamental Trade-Offs

We first consider DST and show that LST can be obtained from DST by replacing the input data \( X \) with \( (Y, S) \).

5.1 Data Space Trade-Off

Consider the optimization problem corresponding to DST in (2). Recall that \( Z = f(X) \) is an \( r \times 1 \) RV, where the embedding dimensionality \( r \) is also a variable to be optimized. A common desiderata of learned representations is that of compactness \([49]\) in order to avoid learning representations with redundant information where different dimensions are highly correlated with each other. Therefore, going beyond the assumption that each component of \( f(\cdot) \) (i.e., \( f_j(\cdot) \)) belongs to a universal RKHS \( H_X \), we impose additional constraints on the representation. Specifically, we constrain the search space of the encoder \( f(\cdot) \) to learn a disentangled representation \([49]\) as follows,

\[
\mathcal{A}_r := \left\{ (f_1, \ldots, f_r) \mid f_i, f_j \in H_X, \mathbb{C}ov_X(f_i(X), f_j(X)) + \gamma \langle f_i, f_j \rangle_{H_X} = \delta_{i,j} \right\}.
\]

In the above set, the \( \mathbb{C}ov(f_i(X), f_j(X)) \) part enforces the covariance of \( Z \) to be an identity matrix. This kind of disentanglement is used in PCA and encourages the variance of each entry of \( Z \) to be bounded and different entries of \( Z \) are uncorrelated to each other. The regularization part, \( \gamma \langle f_i, f_j \rangle_{H_X} \), encourages the encoder components to be as orthogonal as possible to each other and to be of unit norm, and aids with numerical stability during empirical estimation \([50]\). The following theorem shows that such disentanglement is an invertible transformation.

**Theorem 2.** Let \( Z = f(X) \) be an arbitrary representation of the input data \( X \). Then, there exist an invertible measurable function \( t \) such that \( t \circ f \) belongs to \( \mathcal{A}_r \).

This Theorem implies that disentanglement preserves the performance of downstream tasks since target predictors can revert the disentanglement \( t \) and access the original representation \( Z \). In addition, any measurable transformation of \( Z \) will not add any information about \( S \) that does not already exist in \( Z \). The formulation in (2) now reduces to,

\[
\sup_{f \in \mathcal{A}_r} \left\{ J(f(X)) := (1 - \tau) \text{dep}(f(X), Y) - \tau \text{dep}(f(X), S) \right\}, \quad 0 \leq \tau < 1,
\]

where as justified earlier, the target loss function, \( \inf_{g_Y \in H_Y} \mathbb{E}_{X,Y} [L_Y(g_Y(f(X)), Y)] \) can be substituted by \( -\text{dep}(f(X), Y) \). Fortunately, the above optimization problem lends itself to a closed-form solution.
**Theorem 3.** Consider the operator $\Sigma_{SX}$ induced by the linear functional $\text{Cov}(\alpha(X), \beta_S(S)) = \langle \beta_S \Sigma_{SX} \alpha \rangle_{H_S}$ and define $\Sigma_{YX}$ and $\Sigma_{XX}$, similarly. Then, a solution to the formulation in (9) is the eigenfunctions corresponding to $r$ largest eigenvalues of the following generalized problem

$$
(1 - \tau) \Sigma^*_{YX} \Sigma_{YX} - \tau \Sigma^*_{SX} \Sigma_{XS} f = \lambda (\Sigma_{XX} + \gamma I_X) f
$$

where $I_X$ and $\Sigma^*$ are the identity and adjoint operators.

**Remark.** If the trade-off parameter $\tau = 0$ (i.e. no semantic independence constraint is imposed) and $\gamma \to 0$, the solution in Theorem 3 is equivalent to supervised PCA. Similarly, if $\tau \to 1$ (i.e. utility is ignored and only semantic independence is considered), the solution in Theorem 3 is the eigenfunctions corresponding to the negative eigenvalues of $\Sigma^*_{SX} \Sigma_{SX}$, which are the directions that are least explanatory of the semantic attribute $S$.

Now, consider the empirical counterpart of (9),

$$
\sup_{f \in A_r} \left\{ J_{\text{emp}}(f(X)) : = (1 - \tau) \text{dep}_{\text{emp}}(f(X), Y) - \tau \text{dep}_{\text{emp}}(f(X), S) \right\}, \quad 0 \leq \tau < 1
$$

where $\text{dep}_{\text{emp}}(f(X), S)$ and $\text{dep}_{\text{emp}}(f(X), Y)$ are given in (7).

**Theorem 4.** Let the Cholesky factorization be $K_X = L_X L_X^T$, where $L_X \in \mathbb{R}^{n \times l}$ ($l \leq n$) is a full column-rank matrix. A solution to (11) is

$$
f^{opt} = \Theta^{opt} \left[ k_X(x_1, \cdot), \cdots, k_X(x_n, \cdot) \right]^T
$$

where $\Theta^{opt} = U^T(L_X)^\dagger$ and the columns of $U$ are eigenvectors corresponding to $r \leq l$ largest eigenvalues, $\lambda_1, \cdots, \lambda_r \in \Lambda := \{\lambda_1, \cdots, \lambda_l\}$ of the following problem,

$$
L_X^T ((1 - \tau) \tilde{K}_Y - \tau \tilde{K}_S) L_X u = \lambda \left( \frac{1}{n} L_X^T H L_X + \gamma I \right) u
$$

where $\gamma$ is the disentanglement regularization parameter defined in (8) and the supremum value of (11) is $\sum_{j=1}^{r} \lambda_j$.

**Corollary 4.1.** *Embedding Dimensionality*: A useful corollary of Theorem 4 is an optimal embedding dimensionality:

$$
\arg \sup_r \left\{ \sup_{f \in A_r} \left\{ J_{\text{emp}}(f(X)) \right\} \right\},
$$

that is the number of positive eigenvalues in the spectrum $\Lambda = \{\lambda_1, \cdots, \lambda_l\}$.

To examine this result, consider two extreme cases: i) If there is no semantic independence constraint (i.e., $\tau = 0$), adding more dimensions to the optimum $r$ will not harm the representation power of $Z$. ii) If we only care about semantic independence and ignore the target task (i.e., $\tau \to 1$), the optimal $r$ would be equal to zero, indicating that a null representation is the best for discarding all semantic information. In this case, adding more dimension to $Z$ will necessarily violate the semantic independence constraint.

The following Theorem characterizes the convergence of the empirical solution of DST to its population counterpart.

---

3The term solution in any optimization problem in this paper refers to a global optima.
**Theorem 5.** Assume that \( k_S(\cdot, \cdot) \) and \( k_Y(\cdot, \cdot) \) are bounded by one and \( f_j^2(\alpha_i) \leq M \) for any \( j = 1, \ldots, r \) and \( i = 1, \ldots, n \) for which \( f = (f_1, \ldots, f_r) \in A_r \). For any \( n > 1 \) and \( 0 < \delta < 1 \), with probability at least \( 1 - \delta \), we have

\[
\left| \sup_{f \in A_r} J(f(X)) - \sup_{f \in A_r} J_{\text{emp}}(f(X)) \right| \leq rM \sqrt{\frac{\log(6/\delta)}{a^2n}} + O\left(\frac{1}{n}\right),
\]

where \( 0.22 \leq a \leq 1 \) is a constant.

### 5.2 Label Space Trade-Off

Similar to DST, we employ \(-\text{dep}(Z, Y)\) as a proxy for the loss function \( \inf_{g_Y \in H_Y} \mathbb{E}_{X,Y}[L_Y(g_Y(Z), Y)] \).

Recall that LST arises when the representation \( Z \) is ideal and is not a function of \( X \). Then, LST can be formulated as,

\[
\sup_{Z \in L^2_r} \left\{ J(Z) := (1 - \tau) \text{dep}(Z, Y) - \tau \text{dep}(Z, S) \right\},
\]

where \( L^2_r \) is the space of all RVs of dimension \( r \) with finite variance, i.e., \( \mathbb{E}_Z[\|Z - \mathbb{E}[Z]\|^2] < \infty \). Observe from (12) that the optimal \( Z \) is a function of \( p_{Y:S} \) only. Therefore, optimal \( Z \) is of the form,

\[
Z = f_L(Y, S)
\]

where \( f_L(\cdot, \cdot) : \mathbb{R}^{d_Y} \times \mathbb{R}^{d_S} \to \mathbb{R}^r \) is a Borel-measurable function. Instead of directly optimizing \( Z \) over \( L^2_r \), equivalently, we optimize it over all Borel-measurable functions:

\[
\sup_{f_L \in A_r(Y, S)} \left\{ (1 - \tau) \text{dep}(f_L(Y, S), Y) - \tau \text{dep}(f_L(Y, S), S) \right\}
\]

where \( A_r(Y, S) \) is defined similar to \( A_r \) in (8) and replacing \( X \) by \( (Y, S) \). Recall that \( A_r(Y, S) \) ensures the disentanglement of \( Z \) (i.e., compact representation) without affecting invariance or performance of downstream target tasks.

**Remark.** The optimization problem in (14) and its empirical counterpart can be solved similar to that of DST in Theorems 3 and 4 where \( X \) is substituted with \( (Y, S) \).

### 6 Experiments

In this section we numerically quantify the **Label-Space Trade-off** and **Data-Space Trade-off** through the closed-form solutions for the encoder obtained in Section 5 on an illustrative toy example and two large scale datasets, Folktables and CelebA (Section A3 in Appendix), to demonstrate the scalability of our solution.

#### 6.1 Baselines and Implementation Details

**Baselines:** We consider baselines that are based on adversarial representation learning (ARL), the de facto framework for IRL. Specifically, we consider two types of ARL baselines; (1) MSE or Cross-Entropy as the adversarial loss, which only accounts for mean independence (see Sec. I for details) and as such does not account for all modes of dependence. Such methods are expected to fail to learn a fully invariant representation and fail to span the entire DST front. These include ARL [23], SARL [10], and OptNet-ARL [51].

(2)
Adversarial losses that account for all modes of dependence, and as such are expected to, in principle, learn a fully invariant representation and span the entire DST front. These include Wasserstein-ARL [7] and HGR-ARL [52]. Among these baselines, except for SARL and OptNet-ARL, all the others are optimized via iterative minimax optimization which is often unstable and not guaranteed to converge to the global optima. On the other hand, SARL obtains a closed-form solution for the global-optima of the minimax optimization under a linear hypothesis function class, and OptNet-ARL does not involve minimax optimization and learns through standard SGD.

**Implementation Details**: For all methods we pick 100 values of \( \tau \) between zero and one for obtaining the DST and LST. Since the encoder is a neural network in all baseline methods, we train them five times with different random seeds. We let the random seed also change the training-validation-testing split for the Folktables dataset. More implementation details can be found in the appendix (Sec. A).

### 6.2 Datasets and Evaluation Metrics

**Gaussian Toy Example**: We design an illustrative toy example where \( X \) and \( S \) are mean independent but not fully independent. \( X, Y \) and \( S \) are continuous RVs and constructed from the following two independent Gaussian RVs,

\[
U = [U_1, U_2, U_3] \sim \mathcal{N}([0, 0, 0], I_3), \quad N = [N_1, N_2] \sim \mathcal{N}([0, 0], I_2).
\]

Input data is \( X = [X_1, X_2, X_3] \), target and semantic attribute are \( Y = [|U_1|, |U_2|, |U_3|] \) and \( S = [S_1, S_2] \), where

\[
X_1 = \cos \left( \frac{\pi}{6} U_1 \right), \quad [X_2, X_3] = \cos \left( \frac{\pi}{6} [U_2, U_3] \right) + 0.08 N
\]

\[
S_1 = \sin \left( \frac{\pi}{6} U_1 \right), \quad S_2 = \sin \left( \frac{\pi}{6} U_2 \right) + \cos \left( \frac{\pi}{6} U_2 \right)
\]

Since \( S_1 \) and \( S_2 \) are dependent on \( X_1 \) and \( X_2 \), respectively, a totally invariant \( Z \) (i.e., \( Z \perp \perp S \)) should not contain any information about \( X_1 \) and \( X_2 \). However, since \( S_1 \) is only mean independent of \( X_1 \), ARL baselines with MSE based adversary loss i.e., ARL, SARL, OptNet-ARL cannot capture the dependency between \( Z \) to \( X_1 \) and results in a representation that is always partially dependent on \( S_1 \) (see Appendix [II] for more technical details). We sample 18,000 instances from \( p_{X,Y,S} \), independently and split these samples equally into training, validation, and testing datasets.

**Folktables**: We consider fair representation learning on the Folktables [11] dataset, which is a derivation of US Census data from multiple states. We use 2018-Washington Census data with the target attribute \( Y \) as employment status (binary) and the semantic attribute \( S \) as age (continuous value from 0 to 94 years). We seek to learn a representation that predicts employment status while being fair (demographic parity) w.r.t age. It contains 76,225 samples, each with 16 features. We randomly split the data into training (70%), validation (15%), and testing (15%).

**Evaluation Metrics**: For the Gaussian data where the target attribute \( Y \) is a continuous RV, we use MSE as loss function for predicting \( Y \). In this case, utility is defined as,

\[
\text{Utility} := 1 - \frac{\mathbb{E}_{Z,Y}[||\hat{Y} - Y||^2]}{\mathbb{E}_{Z,Y}[||\hat{Y} - \mathbb{E}_Y[Y]||^2]}, \tag{15}
\]

where \( \mathbb{E}_Y[Y] \) is the worst possible prediction of \( Y \) (it occurs when \( Z \) does not contain any information about \( Y \)). We used a kernelized (RBF Gaussian) ridge-regressor to predict \( \hat{Y} \) from \( Z \) for all methods to have a consistent approximation for optimal Bayes regressor. For the Folktables dataset we use accuracy of the
Figure 4: Utility vs semantic dependence trade-offs obtained by our method (LST and DST) and other baselines for Gaussian (a) and Folktables (c) datasets. Comparison of normalized HSIC vs our hybrid dependence measure for (b) Gaussian and (d) Folktables to validate the ability of the latter to account for all modes of dependency between $Z$ and $S$.

binary classification task (employment prediction) as utility. Since HSIC can capture all modes of dependency, we use a normalized version of HSIC, as defined below, to measure the invariance between $Z$ and $S$.

$$\text{NHSIC}(Z, S) := \frac{\text{HSIC}(Z, S)}{\sqrt{\text{HSIC}(Z, Z) \text{HSIC}(S, S)}}$$

6.3 Results

**Fundamental Trade-offs:** Figures 4-a and 4-c show the trade-offs for the Gaussian and Folktables datasets, respectively. We partition the NHSIC values into nine equal intervals between zero and the maximum possible value for NHSICs and compute the mean (solid lines) and standard deviation (shaded regions) of the utility in each interval. We make the following observations, 1) As expected, LST results in 100% utility when $\tau = 0$ i.e., no invariance loss and it outperforms all other trade-offs, both due to its independence from input data $X$ as well as the global optimality of the optimization. LST forms the upper bound that any DST can
aspire to. 2) DST which differs from LST in terms of its dependence on input data $X$. 3) Both LST and DST are highly stable and span the entire trade-off front. 4) The baseline methods, Wasserstein-ARL and HGR-ARL, despite being full dependence measures, lead to sub-optimal DST with large standard deviation due to lack of convergence to global optima and unstable optimization, respectively. 5) The baselines, ARL, SARL and OptNet-ARL, with MSE as the adversary loss span only a very small portion of the trade-off front in the Gaussian example since first dimension of the semantic attribute $S_1$ in (15) is mean independent of $X$, the adversary does not provide any gradients to the encoder to discard $S_1$ from the representation. In both datasets these baselines do not approach $Z \perp \perp S$ i.e., NSHIC=0 for any value of $\tau$.

**Universality of $\text{dep}(Z, S)$:** We empirically examine the practical validity of our assumption in Section 3 and verify if our dependence measure $\text{dep}(Z, S)$, defined in (6), is able to capture all modes of dependency between $Z$ and $S$. Figures 4-b and 4-d shows the plot of the full dependence measure NHSIC vs $\text{dep}$ for the Gaussian and Folktables datasets, respectively. We observe that there is an almost non-decreasing relation between the two measures. And, more importantly as NHSIC($Z, S$) $\to$ 0 so does $\text{dep}(Z, S)$. Together, these observations show that $\text{dep}$ accounts for all modes of dependency between $Z$ and $S$ and the DST obtained by optimizing $\text{dep}$ is equivalent to that obtained by optimizing HSIC.

7 Conclusion

Invariant representation learning often involves trade-offs between utility and semantic dependence. While the existence of such trade-offs and their bounds have been studied, their exact characterization has not been performed. This paper addressed this limitation by, i) exactly establishing two fundamental trade-offs, namely Data-Space Trade-off and Label-Space Trade-off, ii) determining the minimal dimensionality of the representation necessary to achieve a desired optimal trade-off point, and iii) developing a practical and efficient learning algorithm that achieves the exact fundamental trade-off. Specifically, we obtained closed-from solutions for the global optima, both the population and empirical versions, for the underlying optimization problem, and thus characterizing/quantifying the trade-offs exactly. Numerical results on both an illustrative example and real-world datasets show that commonly used adversarial representation learning based techniques are unable to reach the optimal trade-offs estimated by our solution.
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The appendix is organized as follows:

1. Additional experimental details, ablation studies and results on CelebA dataset are provided in Section A.
2. Population Expression for Definition in (6) in Section B.
3. Proof of Lemma 1 in Section C.
4. Proof of Theorem 2 in Section D.
5. Proof of Theorem 3 in Section E.
6. Proofs of Theorem 4 and Corollary 4.1 in Section F.
7. Proof of Theorem 5 in Section G.
8. Justification for substituting utility with dependence measure $dep(Z, Y)$ in Section H.
9. Deficiency of Mean-Squared Error as A Measure of Dependence in Section I.
10. Discussion of limitations of our work in Section J.

A Numerical Evaluation

In this Section we specify all the training details of the numerical results presented in Section 6 of the main paper.

A.1 Gaussian Data

A.1.1 Training Details

LST and DST: We consider RBF Gaussian kernel for $\mathcal{H}_X$, $\mathcal{H}_S$, and linear kernel for $\mathcal{H}_Y$ and we choose the band-width (i.e., $\sigma$) of $\mathcal{H}_X$ and $\mathcal{H}_S$ using the median strategy presented in [53]. We optimize the regularization parameter $\gamma$ in the disentanglement set (8) by minimizing the MSE loss over $\gamma$’s in $\{0, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2}, 10^{-1}, 1\}$ on validation set.

SARL [10]: SARL is similar to our DST except that $\mathcal{H}_S$ is a linear RKHS. We choose $\sigma_X$ and $\gamma$ similar to that of our LST and DST.

ARL [23] and Wass-ARL [7]: The embedding $Z = f(X)$ is extracted via the encoder $f(\cdot)$ which is an MLP with four hidden layers, and 6, 6, 3, and 3 neurons. Then, $Z$ is fed to a target task predictor $g_Y(\cdot)$ and an proxy adversary $g_S(\cdot)$ network where both are MLP with two hidden layers, and 6, 3 neurons. We use stochastic gradient descent-ascent (SGDA) [23] with AdamW [54] as an optimizer to alternately train the encoder, target predictor and proxy adversary networks. We choose the number of epochs and batch-size to be 1200 and 500, respectively, and optimize the learning rate among $\{10^{-2}, 10^{-3}, 3 \times 10^{-4}, 5 \times 10^{-4}, 10^{-4}, 10^{-5}\}$ by minimizing MSE on validation set.

OptNet-ARL [51]: The target and adversary predictors are kernelized ridge regressor with RBF Gaussian kernel of $\sigma_Y = \sigma_X = 1$ as suggested by [51]. The encoder architecture is similar to that of ARL and therefore we follow same training details as ARL.

HGR-ARL [52]: This method is very similar to ARL with the difference that there is a network on the semantic attribute $S$. The encoder and target predictor networks have the same architecture as that of ARL. The adversary network $g_S(\cdot)$ and the network $S$(denoted by $h_S(\cdot)$) are both two-layer MLPs with 6 and 3 neurons. The adversary loss is the correlation coefficients between $g_S(Z)$ and $h_S(S)$. We follow the same optimization procedure as ARL to train the involved neural networks.
Figure 5: Gaussian data: (a) Utility of the target task w.r.t. $\text{dep}(Z, S)$. (b) Utility of the target task w.r.t. $\text{NHSIC}(Z, S)$ for DST with Gaussian, Laplacian, and IMQ kernels.

A.1.2 Effect of Kernel Choice

As an ablation study, we experiment inverse multi-quadratic (IMQ) \cite{55} ($k_X(x, x') = \frac{1}{\sqrt{\|x-x'\|^2 + c}}$) and Laplacian RKHSs ($k_X(x, x') = \exp(-\|x-x'\|/\sigma)$) and compare it with Gaussian RKHS. In this experiment, we let $\mathcal{H}_S$ to be similar to $\mathcal{H}_X$. The results are illustrated in Figure 5-b. We can observe that Laplacian kernel is performing almost similar to Gaussian kernel. On the other hand, IMQ kernel is not performing as good as Gaussian and Laplacian kernels. This is not surprising since IMQ is not a universal kernel.

A.2 Folktables

A.2.1 Training Details

**LST and DST**: We consider RBF Gaussian kernel for $\mathcal{H}_X$, $\mathcal{H}_S$, and linear kernel for $\mathcal{H}_Y$. Since the Folktables is quite a large dataset, we adopt random Features (RF) \cite{56} to obtain finite dimensional feature maps $L_X \in \mathbb{R}^{n \times D_X}$ and $L_S \in \mathbb{R}^{n \times D_S}$. These RFs provide unbiased estimations for kernel matrices (i.e., $K_X \approx L_X L_X^T$ and $K_S \approx L_S L_S^T$) and enable us to use some fast and memory efficient linear approaches for finding optimal $Z$ in Theorem 4 and equation (14) for DST and LST, respectively. We choose the band-width (i.e., $\sigma$) of $\mathcal{H}_X$ and $\mathcal{H}_S$ using the median strategy presented in \cite{53}. The regularization parameter $\gamma$ in the disentanglement set (8) is optimized similar to the experiment on Gaussian data.

**SARL**: SARL is similar to our DST except that $\mathcal{H}_S$ is a linear RKHS. We choose $\sigma_X$ and $\gamma$ similar to that of our LST and DST.

**ARL and Wass-ARL**: The embedding $Z = f(X)$ is extracted via the encoder $f(\cdot)$ which is an MLP with three hidden layers, and 128, 64, and 1 neurons. Then, $Z$ is fed to a target task predictor $g_Y(\cdot)$ and a proxy adversary $g_S(\cdot)$ network where both are MLP with two hidden layers, and 128, 64 neurons. We use SGDA with AdamW as an optimizer to alternately train the encoder, target predictor and proxy adversary networks. We choose the number of epochs and batch-size to be 30 and 128, respectively, and optimize the learning rate among $\{10^{-2}, 10^{-3}, 3 \times 10^{-4}, 5 \times 10^{-4}, 10^{-4}, 10^{-5}\}$ by minimizing MSE in the validation set.

**OptNet-ARL**: The target and adversary predictors are kernelized ridge regressor with RBF Gaussian kernel of $\sigma_Y = \sigma_X = 1$ as suggested by \cite{51}. The encoder architecture is similar to that of ARL and therefore
Figure 6: (a) Accuracy of employment prediction versus \( \text{dep}(Z, S) \). (b) Accuracy of predicting high cheek-bone versus the invariance to gender and age on CelebA dataset.

we follow same training details as ARL.

**HGR-ARL:** This method is very similar to ARL with the difference that there is also a neural network on the semantic attribute \( S \). The encoder and target predictor networks have the same architecture as that of ARL. The adversary network \( g_S(\cdot) \) and the network on \( S \) (denoted by \( h_S(\cdot) \)) are both two-layer MLPs with 2 and 1 neurons. The adversary loss is the correlation coefficients between \( g_S(Z) \) and \( h_S(S) \). We follow the same optimization procedure as ARL to train the involved neural networks.

### A.3 CelebA

CelebA dataset [12] contains 202,599 face images of 10,177 different celebrities with a standard training (162770), validation (19867) and testing (19962) split. Each image is annotated with 40 different attributes. We aim to learn a fair prediction in the sense of demographic parity (DP), defined in [57]. The target task is predicting the high cheek-bone where the sensitive attributes are gender and age. Similar to [58], we deploy DP violation (DPV):

\[
\text{DPV}(\hat{Y}, S) = \max_{S_0, S_0'} \left| P[\hat{Y} | S = S_0] - P[\hat{Y} | S = S_0'] \right|
\]  

(17)

to measure the unfairness (aka invariance) of the prediction \( \hat{Y} \) to gender and age.

We refer to Section 6 of the main paper on choosing the trade-off parameter \( \tau \) and other training settings.

**LST, DST, and SARL:** See the experiment on Gaussian data.

**ARL:** The embedding \( Z = f(X) \) is extracted via the encoder \( f(\cdot) \) which is an MLP with three hidden layers, and 128, 64, and 1 neurons. Then, \( Z \) is fed to a target task predictor \( g_Y(\cdot) \) and an proxy adversary \( g_S(\cdot) \) network where both are MLP with two hidden layers, and 128, 64 neurons. We use SGDA with AdamW as an optimizer to alternately train the encoder, target predictor and proxy adversary networks. We choose the number of epochs and batch-size to be 30 and 128, respectively, and optimize the learning rate among \( \{10^{-2}, 10^{-3}, 3 \times 10^{-4}, 5 \times 10^{-4}, 10^{-4}, 10^{-5}\} \) by minimizing CE in the validation set. We use \( \hat{Y} = g_Y(Z) \) as the prediction of \( Y \).

**OptNet-ARL:** The target and adversary predictors are kernelized ridge regressor with RBF Gaussian kernel of \( \sigma_Y = \sigma_X = 1 \). The encoder architecture is similar to that of ARL and therefore we follow same training details as ARL. After learning the representation \( Z \), we train a two-layer MLP with 128, 64 neurons to predict \( Y \).

**HGR-ARL:** This method is very similar to ARL with the difference that there is also a neural network on the semantic attribute \( S \). The encoder and target predictor networks have the same architecture as that of
ARL. The adversary network $g_S(\cdot)$ and the network on $S$ (denoted by $h_S(\cdot)$) are both two-layer MLPs with 2 and 1 neurons. The adversary loss is the correlation coefficients between $g_S(Z)$ and $h_S(S)$. We follow the same optimization procedure as ARL to train the involved neural networks. Similar to ARL, we use $\hat{Y} = g_Y(Z)$ as the prediction of $Y$.

**Results:** The accuracy of target task versus DPV$(\hat{Y}, S)$ for all methods are illustrated in Figure 6-b. LST is outperforming all other methods. Both DST and SARL are outperforming other baseline methods (except LST) for DPV values closer to zero.
A Population Expression for Definition in (6)

A population expression for \( \text{dep}(Z, S) \) in (6) is given in the following.

\[
\text{dep}(Z, S) = \sum_{j=1}^{r} \left\{ \mathbb{E}_{X,S,X',S'} \left[ f_j(X) f_j(X') k_S(X, X') \right] + \mathbb{E}_X \left[ f_j(X) \right] \mathbb{E}_{X'} \left[ f_j(X') \right] \mathbb{E}_{S,S'} \left[ k_S(X, S') \right] \right. \\
\left. -2 \mathbb{E}_{X,S} \left[ f_j(X) \mathbb{E}_{X'} \left[ f_j(X') \right] \mathbb{E}_{S'} \left[ k_S(S, X') \right] \right] \right\}
\]

where \((X', S')\) is independent of \((X, S)\) with the same distribution as \(p_{X,S}\).

**Proof.** We first note that this population expression is inspired by HSIC [44].

Consider the operator \(\Sigma_{S\chi}\) induced by the linear functional \(\text{Cov}(\alpha(X), \beta_S(S)) = \langle \beta_S, \Sigma_{S\chi} \alpha \rangle_{\mathcal{H}_S}\). Then, it follows that

\[
\text{dep}(Z, S) = \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} \text{Cov}^2 \left( f_j(X), \beta_S(S) \right)
\]

\[
= \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} \langle \beta_S, \Sigma_{S\chi} f_j \rangle^2_{\mathcal{H}_S}
\]

\[
= \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} \langle \beta_S, \Sigma_{S\chi} f_j \rangle^2_{\mathcal{H}_S}
\]

\[
\text{(a)} \sum_{j=1}^{r} \|\Sigma_{S\chi} f_j\|^2_{\mathcal{H}_S}
\]

\[
= \sum_{j=1}^{r} \langle \Sigma_{S\chi} f_j, \Sigma_{S\chi} f_j \rangle_{\mathcal{H}_S}
\]

\[
\text{(b)} \sum_{j=1}^{r} \text{Cov}_{X,S} \left( f_j(X), (\Sigma_{S\chi} f_j)(S) \right)
\]

\[
= \sum_{j=1}^{r} \text{Cov}_{X,S} \left( f_j(X), \langle k_S(\cdot, S), \Sigma_{S\chi} f_j \rangle_{\mathcal{H}_S} \right)
\]

\[
= \sum_{j=1}^{r} \text{Cov}_{X,S} \left( f_j(X), \text{Cov}_{X',S'}(f_j(X'), k_S(S', S)) \right)
\]

\[
= \sum_{j=1}^{r} \text{Cov}_{X,S} \left( f_j(X), \mathbb{E}_{X',S'}[f_j(X') k_S(S, S')] - \mathbb{E}_{X'}[f_j(X')] \mathbb{E}_{S'}[k_S(S, S')] \right)
\]

\[
= \sum_{j=1}^{r} \left\{ \mathbb{E}_{X,S,X',S'} \left[ f_j(X) f_j(X') k_S(S, S') \right] + \mathbb{E}_X \left[ f_j(X) \right] \mathbb{E}_{X'} \left[ f_j(X') \right] \mathbb{E}_{S,S'} \left[ k_S(S, S') \right] \\
-2 \mathbb{E}_{X,S} \left[ f_j(X) \mathbb{E}_{X'} \left[ f_j(X') \right] \mathbb{E}_{S'} \left[ k_S(S, S') \right] \right] \right\}
\]

where (a) is due to Parseval relation for orthonormal basis and (b) is from the definition of \(\Sigma_{S\chi}\).
C Proof of Lemma

Lemma 1. Let $K_X, K_S \in \mathbb{R}^{n \times n}$ be Gram matrices corresponding to $\mathcal{H}_X$ and $\mathcal{H}_S$, respectively, i.e. $(K_X)_{ij} = k_X(x_i, x_j)$ and $(K_S)_{ij} = k_S(s_i, s_j)$. Consider an empirical estimation of covariance as
\[
\text{Cov}(f_j(X), \beta_S(S)) \approx \frac{1}{n} \sum_{i=1}^{n} f_j(x_i) \beta_S(s_i) - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} f_j(x_i) \beta_S(s_k).
\]

It follows that, an empirical estimation for $\text{dep}(Z, S)$ is
\[
\text{dep}_{\text{emp}}(Z, S) := \frac{1}{n^2} \| \Theta K_X HL S \|_F^2,
\]
where $H = I_n - \frac{1}{n} 1_n 1_n^T$ is the centering matrix, and $L_S$ is a full column-rank matrix in which $L_S L_S^T = K_S$ (Cholesky factorization). The empirical estimator in (7) has a bias of $O(n^{-1})$ and a convergence rate of $O(n^{-1/2})$.

Proof. Firstly, let us reconstruct the orthonormal set $U_S$ through i.i.d. observations $\{s_j\}_{j=1}^n$. Invoking representer theorem, for two arbitrary elements $\beta_i$ and $\beta_m$ of $U_S$, we have
\[
\langle \beta_i, \beta_m \rangle_{\mathcal{H}_S} = \langle \sum_{j=1}^{n} \alpha_j k_S(s_j, \cdot), \sum_{l=1}^{n} \eta_l k_S(s_l, \cdot) \rangle_{\mathcal{H}_S} = \sum_{j=1}^{n} \sum_{l=1}^{n} \alpha_j \eta_l k_S(s_j, s_l) = \alpha^T K_S \eta = \langle L_S^T \alpha, L_S^T \eta \rangle_{\mathbb{R}^q}
\]
where $L_S \in \mathbb{R}^{n \times q}$ is a full column-rank matrix and $K_S = L_S L_S^T$ is the Chelesky factorization. As a result, searching for $\beta_i \in U_S$ would become equivalent to searching for $L_S^T \alpha \in U_q$ where $U_q$ is any complete orthonormal set for $\mathbb{R}^q$. Using empirical expression for covariance, we get
\[
\text{dep}_{\text{emp}}(Z, S) := \sum_{\beta_S \in U_S} \sum_{j=1}^{r} \left( \frac{1}{n} \sum_{i=1}^{n} f_j(x_i) \beta_S(s_i) - \frac{1}{n^2} \sum_{i=1}^{n} \sum_{k=1}^{n} f_j(x_i) \beta_S(s_k) \right)^2
\]
\[
= \sum_{L_S^T \alpha \in U_q} \sum_{j=1}^{r} \left( \frac{1}{n} \theta_j^T K_X H K_S \alpha - \frac{1}{n^2} \theta_k^T K_X 1_n 1_n^T K_S \alpha \right)^2
\]
\[
= \sum_{L_S^T \alpha \in U_q} \sum_{j=1}^{r} \left( \frac{1}{n} \theta_j^T K_X H L_S L_S^T \alpha \right)^2
\]
\[
= \sum_{\zeta \in U_q} \sum_{j=1}^{r} \left( \frac{1}{n} \theta_j^T K_X H L_S \zeta \right)^2
\]
\[
= \sum_{\zeta \in U_q} \frac{1}{n^2} \| \Theta K_X H L_S \zeta \|_2^2
\]
\[
= \frac{1}{n^2} \| \Theta K_X H L_S \|_F^2,
\]
where \( f(X) = \Theta [k_X(x_1, X), \ldots, k_X(x_n, X)]^T \) and \( \Theta := [\theta_1, \ldots, \theta_r]^T \).

We now show that the bias of \( \text{dep}^{epm}(Z, S) \) to estimate \( \text{dep}(Z, S) \) in (7) is \( \mathcal{O}(\frac{1}{n^3}) \). To do this, we split \( \text{dep}^{epm}(Z, S) \) into three terms as

\[
\frac{1}{n^2} \| \Theta K_X H^T S \|_F^2 = \frac{1}{n^2} \text{Tr}\left\{ \Theta K_X H K_X H^T \Theta^T \right\} = \frac{1}{n^2} \text{Tr}\left\{ \Theta K_X \left( I - \frac{1}{n} 11^T \right) K_S \left( I - \frac{1}{n} 11^T \right) K_X \Theta^T \right\} = \frac{1}{n^2} \text{Tr}\left\{ K_X \Theta^T K_X K_S \right\} - \frac{2}{n^3} \text{Tr}\left\{ 1^T K_X \Theta^T K_X K_S 1 \right\} + \frac{1}{n^4} \text{Tr}\left\{ 1^T K_X \Theta^T K_X 11^T K_S 1 \right\}
\]

Let \( c^n_p \) denote the set of all \( p \)-tuples drawn without repetition from \( \{1, \ldots, n\} \). Also, let \( \Theta = [\theta_1, \ldots, \theta_r]^T \in \mathbb{R}^{r \times n} \) and \((A)_{ij}\) denote the element of arbitrary matrix \( A \) at \( i \)’th row and \( j \)’th column. Then, it follows that

(I):

\[
\mathbb{E}\left[ \text{Tr}\left\{ K_X \Theta^T K_X K_S \right\} \right] = \sum_{k=1}^{r} \mathbb{E}\left[ \text{Tr}\left\{ K_X \theta_k \theta_k^T K_X K_S \right\} \right] = \sum_{k=1}^{r} \mathbb{E}\left[ \text{Tr}\left\{ \alpha_k \alpha_k^T K_S \right\} \right] = \sum_{k=1}^{r} \mathbb{E}\left[ \sum_{i}(\alpha_k \alpha_k^T)_{ii}(K_S)_{ii} + \sum_{(i,j) \in c^n_2} (\alpha_k \alpha_k^T)_{ij}(K_S)_{ij} \right] = n \sum_{k=1}^{r} \mathbb{E}_{X,S}\left[ f_k^2(X)k_S(S, S) \right] + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'}\left[ f_k(X)f_k(X')k_S(S, S') \right] = \mathcal{O}(n) + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'}\left[ f_k(X)f_k(X')k_S(S, S') \right]
\]

(II):

\[
\mathbb{E}\left[ 1^T K_X \Theta^T K_X K_S 1 \right] = \sum_{k=1}^{r} \mathbb{E}\left[ 1^T K_X \theta_k \theta_k^T K_X K_S 1 \right] = \sum_{k=1}^{r} \mathbb{E}\left[ 1^T \alpha_k \alpha_k^T K_S 1 \right] = \sum_{k=1}^{r} \mathbb{E}\left[ \sum_{m=1}^{n} \sum_{i=1}^{n} \sum_{j=1}^{n} (\alpha_k \alpha_k^T)_{mi}(K_S)_{mj} \right]
\]
\begin{align*}
&= \sum_{k=1}^{r} \mathbb{E} \left[ \sum_{i} (\alpha_k \alpha_k^T)_{ii} (K_S)_{ii} + \sum_{(m,j) \in e_2^r} (\alpha_k \alpha_k^T)_{mm} (K_S)_{mj} \right] \\
&\quad + \sum_{k=1}^{r} \mathbb{E} \left[ \sum_{(m,i) \in e_2^r} (\alpha_k \alpha_k^T)_{mi} (K_S)_{mm} + \sum_{(m,j) \in e_2^r} (\alpha_k \alpha_k^T)_{mj} (K_S)_{mj} \right] \\
&\quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad + \sum_{k=1}^{r} \mathbb{E} \left[ \sum_{(m,i,j) \in e_3^r} (\alpha_k \alpha_k^T)_{mi} (K_S)_{mj} \right] \\
&= n \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k^2(X) k_S(S,S) \right] + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,S'} \left[ f_k^2(X) k_S(S,S') \right] \\
&\quad + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X'} \left[ f_k(X) f_k(X') k_S(S,S) \right] \\
&\quad + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'} \left[ f_k(X) f_k(X') k_S(S,S') \right] \\
&\quad + \frac{n!}{(n-3)!} \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k(X) \mathbb{E}_{X'}[f_k(X')] \mathbb{E}_{S'}[k_S(S,S')] \right] \\
&= O(n^2) + \frac{n!}{(n-3)!} \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k(X) \mathbb{E}_{X'}[f_k(X')] \mathbb{E}_{S'}[k_S(S,S')] \right]. \quad (21)
\end{align*}

(III):

\begin{align*}
\mathbb{E} \left[ 1^T K_X \Theta^T \Theta K_X 11^T K_S 1 \right] &= \sum_{k=1}^{r} \mathbb{E} \left[ 1^T K_X \theta_k \theta_k^T K_X 11^T K_S 1 \right] \\
&= \sum_{k=1}^{r} \mathbb{E} \left[ 1^T \alpha_k \alpha_k^T 11^T K_S 1 \right] \\
&= \sum_{k=1}^{r} \mathbb{E} \left[ \sum_{i,j,m,l} (\alpha_k \alpha_k^T)_{ij} (K_S)_{ml} \right] \\
&= O(n^3) + \sum_{k=1}^{r} \mathbb{E} \left[ \sum_{(i,j,m,l) \in e_4^r} (\alpha_k \alpha_k^T)_{ij} (K_S)_{ml} \right] \\
&= O(n^3) + \frac{n!}{(n-4)!} \sum_{k=1}^{r} \mathbb{E}_{X} \left[ f_k(X) \right] \mathbb{E}_{X'} \left[ f_k(X') \right] \mathbb{E}_{S,S'} \left[ k_S(S,S') \right].
\end{align*}

(22)

Using above calculations together with Lemma 2 lead to

\[ \text{dep}(Z, S) \leq \mathbb{E} \left[ \text{dep}^{\text{emp}}(Z, S) \right] + O \left( \frac{1}{n} \right). \]

We now obtain the convergence of \( \text{dep}^{\text{emp}}(Z, S) \). Consider the decomposition in (19) together with (20), (21), and (22). Let \( \alpha_k := K_X \theta_k \), then it follows that

\[ \mathbb{P} \left\{ \text{dep}(Z, S) - \text{dep}^{\text{emp}}(Z, S) \geq t \right\} \]
\[
\begin{align*}
&\leq \mathbb{P}\left\{ \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'} [f_k(X)f_k(X')k_S(S',S')] - \frac{(n-2)!}{n!} \sum_{k=1}^{r} \sum_{(i,j) \in e^2_k} (\alpha_k \alpha_k^T)_{ij}(K_S)_{ij} + \mathcal{O}\left(\frac{1}{n}\right) \geq at \right\} \\
&+ \mathbb{P}\left\{ \sum_{k=1}^{r} \mathbb{E}_{X,S} [f_k(X)\mathbb{E}_{X'}[f_k(X')]\mathbb{E}_{S'}[k_S(S',S')]] - \frac{(n-3)!}{n!} \sum_{k=1}^{r} \sum_{(i,j,m) \in e^2_k} (\alpha_k \alpha_k^T)_{mi}(K_S)_{mj} + \mathcal{O}\left(\frac{1}{n}\right) \geq bt \right\} \\
&+ \mathbb{P}\left\{ \sum_{k=1}^{r} \mathbb{E}_{X} [f_k(X)\mathbb{E}_{X'}[f_k(X')]\mathbb{E}_{S,S'}[k_S(S,S')]] - \frac{(n-4)!}{n!} \sum_{k=1}^{r} \sum_{(i,j,m,l) \in e^2_k} (\alpha_k \alpha_k^T)_{ij}(K_S)_{ml} + \mathcal{O}\left(\frac{1}{n}\right) \geq (1-a-b)t \right\},
\end{align*}
\]

where \(a, b > 0\) and \(a + b < 1\). For convenience, we omit the term \(\mathcal{O}\left(\frac{1}{n}\right)\) and add it back in the last stage.

Define \(\zeta := (X, S)\) and consider the following U-statistics \([59]\)

\[
\begin{align*}
(u_1)_{ij} &= \frac{(n-2)!}{n!} \sum_{(i,j) \in e^2_k} \sum_{k=1}^{r} (\alpha_k \alpha_k^T)_{ij}(K_S)_{ij} \\
(u_2)_{ij} &= \frac{(n-3)!}{n!} \sum_{(i,j,m) \in e^2_k} \sum_{k=1}^{r} (\alpha_k \alpha_k^T)_{mi}(K_S)_{mj} \\
(u_3)_{ij} &= \frac{(n-4)!}{n!} \sum_{(i,j,m,l) \in e^2_k} \sum_{k=1}^{r} (\alpha_k \alpha_k^T)_{ij}(K_S)_{ml}
\end{align*}
\]

Then, from Hoeffding’s inequality \([59]\) it follows that

\[
\mathbb{P}\left\{ \left| \text{dep}(Z, S) - \text{dep}^{\text{emp}}(Z, S) \right| \geq t \right\} \leq e^{-\frac{2a^2t^2}{2r^2M^2n}} + e^{-\frac{2b^2t^2}{3r^2M^2n}} + e^{-\frac{2(1-a-b)^2t^2}{4r^2M^2n}},
\]

where we assumed that \(k_S(\cdot, \cdot)\) is bounded by one and \(f_k^2(X_i)\) is bounded by \(M\) for any \(k = 1, \ldots, r\) and \(i = 1, \ldots, n\).

Further, if \(0.22 \leq a < 1\), it holds that

\[
\frac{-2a^2t^2}{e^{2r^2M^2n}} + e^{-\frac{2b^2t^2}{3r^2M^2n}} + e^{-\frac{2(1-a-b)^2t^2}{4r^2M^2n}} \leq 3e^{-\frac{a^2t^2}{2r^2M^2n}}.
\]

Consequently, we have

\[
\mathbb{P}\left\{ \left| \text{dep}(Z, S) - \text{dep}^{\text{emp}}(Z, S) \right| \geq t \right\} \leq 6e^{-\frac{a^2t^2}{2r^2M^2n}}.
\]

Therefore, with probability at least \(1 - \delta\), it holds

\[
\left| \text{dep}(Z, S) - \text{dep}^{\text{emp}}(Z, S) \right| \leq \sqrt{\frac{r^2M^2\log(6/\sigma)}{\alpha^2n}} + \mathcal{O}\left(\frac{1}{n}\right).
\]
D Proof of Theorem 2

Theorem 2. Let $Z = f(X)$ be an arbitrary representation of the input data $X$. Then, there exist an invertible measurable function $t$ such that $t \circ f$ belongs to $A_r$.

Proof. Recall that the space of disentangled representation is

$$A_r := \left\{ (f_1, \cdots, f_r) \mid f_i, f_j \in \mathcal{H}_X, \text{Cov}_X (f_i(X), f_j(X)) + \gamma (f_i, f_j)_{\mathcal{H}_X} = \delta_{i,j} \right\},$$

where $\gamma > 0$. Let $I_X$ denote the identity operator from $\mathcal{H}_X$ to $\mathcal{H}_X$. We claim that $t = [t_1, \cdots, t_r]$, where

$$G_0 = \begin{bmatrix} (f_1, f_1)_{\mathcal{H}_X} & \cdots & (f_1, f_r)_{\mathcal{H}_X} \\ \vdots & \ddots & \vdots \\ (f_r, f_1)_{\mathcal{H}_X} & \cdots & (f_r, f_r)_{\mathcal{H}_X} \end{bmatrix}$$

$$G = G_0^{-1/2}$$

$$t_j \circ f = \sum_{m=1}^r g_{j,m} (\Sigma_{XX} + \gamma I_X)^{-1/2} f_j, \quad \forall j = 1, \cdots, r$$

is the desired transformation. To see this, construct

$$\text{Cov}_X (t_j(f(X)), t_j(f(X))) + \gamma \langle t_i \circ f, t_j \circ f \rangle_{\mathcal{H}_X}$$

$$= \langle t_i \circ f, (\Sigma_{XX} + \gamma I_X) t_j \circ f \rangle_{\mathcal{H}_X}$$

$$= \langle \sum_{m=1}^r g_{i,m} (\Sigma_{XX} + \gamma I_X)^{-1/2} f_i, \sum_{k=1}^r g_{j,k} (\Sigma_{XX} + \gamma I_X) (\Sigma_{XX} + \gamma I_X)^{-1/2} f_j \rangle_{\mathcal{H}_X}$$

$$= \sum_{m=1}^r \sum_{k=1}^r g_{i,m} g_{j,k} \langle f_i, f_j \rangle_{\mathcal{H}_X} = \delta_{i,j}$$

The inverse of $t$ is $t' = [t'_1, \cdots, t'_r]$ where

$$H = G_0^{1/2}$$

$$t'_j \circ t = \sum_{m=1}^r h_{j,m} (\Sigma_{XX} + \gamma I_X)^{1/2} t_j, \quad \forall j = 1, \cdots, r$$

E Proof of Theorem 3

Theorem 3. Consider the operator $\Sigma_{SX}$ induced by the linear functional $\text{Cov}(\alpha(X), \beta_S(S)) = \langle \beta_S \Sigma_{SX} \alpha \rangle_{\mathcal{H}_S}$ and define $\Sigma_{YX}$ and $\Sigma_{XX}$, similarly. Then, a solution to the optimization problem in (9) is the eigenfunctions corresponding to $r$ largest eigenvalues of the following generalized problem

$$\left((1 - \tau) \Sigma_{YX}^* \Sigma_{YX} - \tau \Sigma_{SX}^* \Sigma_{XX} \right) f = \lambda (\Sigma_{XX} + \gamma I_X) f,$$

where $I_X$ is the identity operator from $I_X$ to $I_X$ and $\Sigma^*$ denotes the adjoint operator.
\[ \text{Proof. Consider dep}(Z, S) \text{ in (6)}:\]
\[
\text{dep}(Z, S) = \sum_{\beta_S \in \mathcal{U}_S} \sum_{j=1}^r \text{Cov}^2(f_j(X), \beta_S(S))
\]
\[
= \sum_{j=1}^r \sum_{\beta_S \in \mathcal{U}_S} \left< \beta_S, \Sigma_{SX} f_j \right>^2_{\mathcal{H}_S}
\]
\[
= \sum_{j=1}^r \| \Sigma_{SX} f_j \|^2_{\mathcal{H}_S},
\]
where the last step is due to Parseval’s identity for orthonormal basis. Similarly, we have \( \text{dep}(Z, Y) = \sum_{j=1}^r \| \Sigma_{XY} f_j \|^2_{\mathcal{H}_Y}. \)
Recall that \( Z = f(X) = (f_1(X), \cdots, f_r(X)) \), then, it follows that
\[
J(f(X)) = (1 - \tau) \sum_{j=1}^r \| \Sigma_{XY} f_j \|^2_{\mathcal{H}_Y} - \tau \sum_{j=1}^r \| \Sigma_{SX} f_j \|^2_{\mathcal{H}_S}
\]
\[
= (1 - \tau) \sum_{j=1}^r \left< \Sigma_{XY} f_j, \Sigma_{XY} f_j \right>_{\mathcal{H}_Y} - \tau \sum_{j=1}^r \left< \Sigma_{SX} f_j, \Sigma_{SX} f_j \right>_{\mathcal{H}_S}
\]
\[
= \sum_{j=1}^r \left< f_j, (1 - \tau) \Sigma^*_X \Sigma_{XY} - \tau \Sigma^*_X \Sigma_{SX} \right>_{\mathcal{H}_X},
\]
where \( \Sigma^* \) is the adjoint operator of \( \Sigma. \) Further, note that \( \text{Cov}_X(f_i(X), f_j(X)) = \left< f_i, \Sigma_{XX} f_j \right>_{\mathcal{H}_X}. \) As a result, the optimization problem in (11) can be restated as
\[
\sup_{\langle f_i, (\Sigma_{XX} + \gamma I_X) f_k \rangle_{\mathcal{H}_X} = \delta_{i,k}} \sum_{j=1}^r \left< f_j, (1 - \tau) \Sigma^*_X \Sigma_{XY} - \tau \Sigma^*_X \Sigma_{SX} \right>_{\mathcal{H}_X}, \quad 1 \leq i, k \leq r
\]
where \( I_X \) denotes identity operator from \( \mathcal{H}_X \) to \( \mathcal{H}_X. \) This optimization problem is known as generalized Rayleigh quotient \([60]\) and a possible solution to it is given by the eigenfunctions corresponding to the \( r \) largest eigenvalues of the following generalized problem
\[
(1 - \tau) \Sigma_{XY} \Sigma_{XY} - \tau \Sigma_{SX} \Sigma_{SX} f = \lambda \left( \Sigma_{XX} + \gamma I_X \right) f.
\]
\[ \square \]

\section{Proofs of Theorem 4 and Corollary 4.1}

\textbf{Theorem 4.} Let the Cholesky factorization be \( K_X = L_X L_X^T, \) where \( L_X \in \mathbb{R}^{n \times l} \) \((l \leq n)\) is a full column-rank matrix. A solution to \( \Pi \) is
\[
f^{\text{opt}} = \Theta^{\text{opt}} \left[ k_X(x_1, \cdot), \cdots, k_X(x_n, \cdot) \right]^T
\]
where \( \Theta^{\text{opt}} = U^T(L_X)^T \) and the columns of \( U \) are eigenvectors corresponding to \( r \leq l \) largest eigenvalues, \( \lambda_1, \cdots, \lambda_r \in \Lambda := \{\lambda_1, \cdots, \lambda_l\} \) of the following generalized problem,
\[
L_X^T ((1 - \tau) \tilde{K}_Y - \tau \tilde{K}_S) L_X U = \lambda \left( \frac{1}{n} L_X^T H L_X + \gamma I \right) U
\]
where \( \gamma \) is the disentanglement regularization parameter defined in \( [8] \) and the supremum value of \( \Pi \) is \( \sum_{j=1}^r \lambda_j. \)
Proof. Consider the Cholesky factorization $K_x = L_x L_x^T$ where $L_x$ is a full row-rank matrix. Using representer theorem, disentanglement condition in (10), can be expressed as

$$\text{Cov}(f_i(X), f_j(X)) + \gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}$$

$$= \frac{1}{n} \sum_{k=1}^{n} f_i(X_k) f_j(X_k) - \frac{1}{n^2} \sum_{k=1}^{n} f_i(X_k) \sum_{m=1}^{n} f_j(X_m) + \gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}$$

$$= \frac{1}{n} \sum_{k=1}^{n} \sum_{l=1}^{n} K_X(X_k, X_l) \theta_{il} \sum_{m=1}^{n} K_X(X_k, X_m) \theta_{jm} - \frac{1}{n^2} \theta_i^T K_X 1_n 1_n^T K_X \theta_j + \gamma \langle \sum_{k=1}^{n} \theta_{ik} k_X(\cdot, X_k), \sum_{l=1}^{n} \theta_{il} k_X(\cdot, X_l) \rangle_{\mathcal{H}_X}$$

$$= \frac{1}{n} (K_X \theta_i)^T (K_X \theta_j) - \frac{1}{n^2} \theta_i^T K_X 1_n 1_n^T K_X \theta_j + \gamma \langle \sum_{k=1}^{n} \theta_{ik} k_X(\cdot, X_k), \sum_{l=1}^{n} \theta_{il} k_X(\cdot, X_l) \rangle_{\mathcal{H}_X}$$

$$= \frac{1}{n} \theta_i^T K_X H K_X \theta_j + \gamma \theta_i^T K_X \theta_j$$

$$= \frac{1}{n} \theta_i^T L_X \left( L_X^T H L_X + n \gamma I \right) L_X^T \theta_j$$

$$= \delta_{i,j}.$$ 

As a result, $f \in \mathcal{A}_r$ is equivalent to

$$\Theta L_X \left( \frac{1}{n} L_X^T H L_X + n \gamma I \right) L_X^T \Theta^T = I_r,$$

where $\Theta := [\theta_1, \ldots, \theta_r]^T \in \mathbb{R}^{r \times n}$. Let $V = L_X^T \Theta$ and consider the optimization problem in (13):

$$\sup_{f \in \mathcal{A}_r} \left\{ (1 - \tau) \text{dep}_{\text{emp}}(f(X), Y) - \tau \text{dep}_{\text{emp}}(f(X), S) \right\}$$

$$= \sup_{f \in \mathcal{A}_r} \frac{1}{n^2} \left\{ (1 - \tau) \| \Theta K_X H L_Y \|_F^2 - \tau \| \Theta K_X H L_S \|_F^2 \right\}$$

$$= \sup_{f \in \mathcal{A}_r} \frac{1}{n^2} \left\{ (1 - \tau) \text{Tr} \left\{ \Theta K_X H K_Y H K_X \Theta^T \right\} - \tau \text{Tr} \left\{ \Theta K_X H K_S H K_X \Theta^T \right\} \right\}$$

$$= \max_{V^T CV = I_r} \frac{1}{n^2} \text{Tr} \left\{ \Theta L_X B L_X^T \Theta^T \right\}$$

$$= \max_{V^T CV = I_r} \frac{1}{n^2} \text{Tr} \left\{ V^T B V \right\}$$

(24)

where the second step is due to \cite{7} and \cite{6}. It is shown in \cite{61} that an optimizer of (24) is any matrix $U$ whose columns are eigenvectors corresponding to $r$ largest eigenvalues of generalized problem

$$B u = \lambda C u$$

(25)

\footnote{Optimal $V$ is not unique.}
and the maximum value is the summation of $r$ largest eigenvalues. Once $U$ is determined, then, any $\Theta$ in which $L_X^T \Theta^T = U$ is optimal $\Theta$ (denoted by $\Theta_{\text{opt}}$). Note that $\Theta_{\text{opt}}$ is not unique and has a general form of

$$\Theta^T = (L_X^T)^\dagger U + \Lambda_0, \quad \mathcal{R}(\Lambda_0) \subseteq \mathcal{N}(L_X^T).$$

However, setting $\Lambda_0$ to zero would lead to minimum norm for $\Theta$. Therefore, we opt $\Theta_{\text{opt}} = U^T (L_X)^\dagger$.

**Corollary 4.1. Embedding Dimensionality:** A useful corollary of Theorem 4 is an optimal embedding dimensionality:

$$\arg\sup_r \left\{ \sup_{f \in A_r} \left\{ J_{\text{emp}}(f(X)) \right\} \right\},$$

that is the number of positive eigenvalues in the spectrum $\Lambda = \{\lambda_1, \ldots, \lambda_l\}$.

**Proof.** From the proof of Theorem 5, we know that

$$\sup_{f \in A_r} \left\{ (1 - \tau) \text{dep}^\text{emp}(f(X), Y) - \tau \text{dep}^\text{emp}(f(X), S) \right\} = \sum_{j=1}^r \lambda_j,$$

where $\{\lambda_1, \ldots, \lambda_l\}$ are eigenvalues of the generalized problem in (12) in decreasing order. It follows immediately that

$$\arg\sup_r \left\{ \sum_{j=1}^r \lambda_j \right\} = \text{number of positive elements of } \{\lambda_1, \ldots, \lambda_l\}.$$
Since $J(f(X)) = (1-\tau) \text{dep}(Z, Y) - \tau \text{dep}(Z, S)$ and $J_{\text{emp}}(f(X)) := (1-\tau) \text{dep}_{\text{emp}}(Z, Y) - \tau \text{dep}_{\text{emp}}(Z, S)$, it follows that with probability at least $1 - \delta$,

$$\left| J(f(X)) - J_{\text{emp}}(f(X)) \right| \leq rM \sqrt{\frac{\log(6/\delta)}{\alpha^2 n}} + O\left(\frac{1}{n}\right).$$

We complete the proof by noting that

$$\left| \sup_{f \in \mathcal{A}} J(f(X)) - \sup_{f \in \mathcal{A}} J_{\text{emp}}(f(X)) \right| \leq \sup_{f \in \mathcal{A}} \left| J(f(X)) - J_{\text{emp}}(f(X)) \right|.$$

\[ \Box \]

### H Optimality of Utility in DST

We show that maximizing $\text{dep}(f(X), Y)$ can lead to a representation $Z$ that is sufficient enough to result in the optimal Bayes prediction of $Y$.

**Theorem 6.** Let $\tau = 0$, $\gamma \to 0$, $\mathcal{H}_Y$ be a linear RKHS, and $f^*$ be the concatenation of the eigenfunctions corresponding to $d_Y$ number of largest eigenvalues of the generalized problem in (10). Then, there exist an affine regressor on top of the representation $Z^* = f^*(X)$ that can perform as well as the Bayes regressor $\mathbb{E}_Y[Y|X]$, i.e.

$$\min_{W, b} \mathbb{E}_{X,Y} \left[ \| WZ^* + b - Y \|^2 \right] = \mathbb{E}_{X,Y} \left[ \| \mathbb{E}_Y[Y|X] - Y \|^2 \right].$$

This Theorem implies that not only can $\text{dep}(f(X), Y)$ preserve all the necessary information in $Z^*$ to optimally predict $Y$, the learned representation is also simple enough for a linear regressor to perform as effective as the Bayes regressor $\mathbb{E}_Y[Y|X]$.

**Proof.** We only prove this Theorem for the empirical version due to its convergence to the population counterpart. The optimal Bayes predictor can be the composition of the kernelized encoder $\hat{Z} = f(X)$ and an affine regressor on top of it. More specifically, $\hat{Y} = Wf(X) + b$ can approach to the optimal Bayes predictor if we optimize $f$, $r$ (the dimensionality of $f$), $W$, and $b$ all together. Let $Z := [z_1, \ldots, z_n] \in \mathbb{R}^{d_y \times n}$ and $\hat{Y} := [y_1, \ldots, y_n] \in \mathbb{R}^{d_y \times n}$. Further, let $\tilde{Z}$ and $\tilde{y}$ be the centered (i.e., mean subtracted) version of $Z$ and $\hat{Y}$, respectively. We firstly optimize $b$ for any given $f$, $r$ and $W$:

$$b_{\text{opt}} := \arg \min_b \frac{1}{n} \sum_{i=1}^{n} \| Wz_i + b - y_i \|^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} y_i - W \frac{1}{n} \sum_{i=1}^{n} z_i.$$  

Then, optimizing over $W$ would lead to

$$\min_{W} \frac{1}{n} \| W\tilde{Z} - \tilde{Y} \|_F^2 = \frac{1}{n} \min_{W} \| \tilde{Z}^T W^T - \tilde{Y}^T \|_F^2$$

$$= \frac{1}{n} \min_{W} \| \tilde{Z}^T W^T - P\tilde{Z} \tilde{Y}^T \|_F^2 + \frac{1}{n} \| P\tilde{Z} \tilde{Y}\|_F^2$$

$$= \frac{1}{n} \| P\tilde{Z} \tilde{Y} \|_F^2.$$
where $P_{\tilde{Z}}$ denotes the orthogonal projector onto the columns of $\tilde{Z}^T$ and a possible minimizer is $W_{\text{opt}}^T = (\tilde{Z}^T)^\dagger \tilde{Y}^T$ or equivalently $W_{\text{opt}} = \tilde{Y}(\tilde{Z})^\dagger$. Since the optimal MSE loss is a function of the range (column space) of $\tilde{Z}^T$, we can consider only $\tilde{Z}^T$ with orthonormal columns or equivalently $\frac{1}{n} \tilde{Z} \tilde{Z}^T = I_r$. In this setting it holds $P_{\tilde{Z}} = \frac{1}{n} \tilde{Z} \tilde{Z}^T$. Now, consider optimizing $f(X) = \Theta |k_X(x_1, X), \cdots, k_X(x_n, X)|^T$. We have, $\tilde{Z} = \Theta K_X H$ where $H$ is the centering matrix. Let $V = L_X^T \Theta^T$ and $C = \frac{1}{n} L_X^T H L_X$

$$
\begin{align*}
\min_{\Theta K_X H K_X \Theta^T = \Theta K_X H K_X \Theta^T = I_r, n} & n \left\{ \frac{1}{n} \| \tilde{Y}^\prime \|_F^2 - \| P_{\tilde{Z}} \tilde{Y}^\prime^T \|_F^2 \right\} \\
= & \frac{1}{n} \| \tilde{Y}^\prime \|_F^2 - \max_{\Theta K_X H K_X \Theta^T = \Theta K_X H K_X \Theta^T = I_r, n} \frac{1}{n} \| P_{\tilde{Z}} \tilde{Y}^\prime^T \|_F^2 \\
= & \frac{1}{n} \| \tilde{Y}^\prime \|_F^2 - \max_{V^T CV = I_r, n^2} \frac{1}{n^2} \text{Tr} \left[ \tilde{Y} H K_X \Theta^T \Theta K_X H \tilde{Y}^T \right] \\
= & \frac{1}{n^2} \| \tilde{Y}^\prime \|_F^2 - \max_{V^T CV = I_r, n^2} \frac{1}{n^2} \text{Tr} \left[ \Theta K_X H \tilde{Y}^T \tilde{Y} \Theta K_X H \Theta^T \right] \\
= & \| \tilde{Y}^\prime \|_F^2 - \frac{1}{n^2} \text{Tr} \left[ V^T L_X^T \tilde{Y}^T \tilde{Y} L_X V \right] \\
= & \frac{1}{n} \| \tilde{Y}^\prime \|_F^2 - \frac{1}{n^2} \sum_{j=1}^r \lambda_j,
\end{align*}
$$

where $\lambda_1, \cdots, \lambda_r$ are $r$ largest eigenvalues of the following generalized problem

$$
B_0 u = \lambda Cu
$$

and $B_0 := L_X^T \tilde{Y}^T \tilde{Y} L_X$. This is resembles the eigenvalue in Section 6 equation (25) where $\tau = 0$, $\mathcal{H}_Y$ is a linear RKHS and $\gamma \to 0$. Further, the number of positive eigenvalues is the rank of $B_0$ which is at most $d_Y$.

I Deficiency of Mean-Squared Error as A Measure of Dependence

**Theorem.** Let $\mathcal{H}_S$ contain all Borel-measurable functions, $S$ be a $d_S$-dimensional RV, and $L_S(\cdot, \cdot)$ be MSE loss. Then,

$$
Z \in \arg\sup \left\{ \inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X, S} \left[ L_S \left( g_S(Z), S \right) \right] \right\} \Leftrightarrow \mathbb{E}[S \mid Z] = \mathbb{E}[S].
$$

**Proof.** Let $S_i$, $(g_S(Z))_i$, and $(\mathbb{E}[S \mid Z])_i$ denote the $i$’th entries of $S$, $g_S(Z)$, and $\mathbb{E}[S \mid Z]$, respectively. Then, it follows that

$$
\begin{align*}
\inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X, S} \left[ L_S \left( g_S(Z), S \right) \right] &= \inf_{g_S \in \mathcal{H}_S} \sum_{i=1}^{d_S} \mathbb{E}_{X, S} \left[ \left( g_S(Z) \right)_i - S_i \right]^2 \\
&= \sum_{i=1}^{d_S} \mathbb{E}_{X, S} \left[ \left( \mathbb{E}[S \mid Z] \right)_i - S_i \right]^2 \\
&\leq \sum_{i=1}^{d_S} \mathbb{E} \left[ \left( \mathbb{E}[S] \right)_i - S_i \right]^2 = \sum_{i=1}^{d_S} \text{Var}[S_i],
\end{align*}
$$

where the second step is due to the optimality of conditional mean (i.e., Bayes estimation) for MSE [62] and the last step is due the fact that independence between $Z$ and $S$ leads to an upper bound on MSE.
Therefore, if \( Z \in \arg \sup \left\{ \inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X,S} \left[ L_S \left( g_S(Z), S \right) \right] \right\} \), then \( \mathbb{E}[S | Z] = \mathbb{E}[S] \). On the other hand, if \( \mathbb{E}[S | Z] = \mathbb{E}[S] \), then it follows immediately that \( Z \in \arg \sup \left\{ \inf_{g_S \in \mathcal{H}_S} \mathbb{E}_{X,S} \left[ L_S \left( g_S(Z), S \right) \right] \right\} \).

This theorem implies that an optimal adversary does not necessarily lead to a representation \( Z \) that is statistically independent of \( S \), but rather leads to \( S \) being mean independent of the representation \( Z \) i.e., independence with respect to first order moment only.

We also note that in the Label-Space Trade-off, when \( L_Y \) is MSE and \( \text{dep}(\cdot, \cdot) \) is the mean dependence between \( Z \) and \( S \) as defined above, the LST reduces to the noiseless setting studied by [8].

### J Discussion and Limitations

We believe that our theoretical results and algorithmic solutions shed light on the regions of the trade-off that are feasible or impossible to achieve by representation learning algorithms for a variety of settings such as algorithmic fairness, privacy-preserving learning, etc. The fundamental trade-offs in IRL are a function of the choice of dependence measures that capture all modes of dependence between two random variables. As such, the trade-offs obtained in this paper are optimal for HSIC like dependence measures. Studying the trade-offs obtained by other full measures of dependence and comparing them the ones obtained in this paper is a promising direction for future work.