On 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 often formulated as satisfying two potentially competing objectives: maximizing utility for predicting a target attribute while simultaneously being independent or invariant with respect to a known semantic attribute. In this paper, we identify and determine two fundamental trade-offs between utility and semantic dependence induced by the statistical dependencies between the data and its corresponding target and semantic attributes. We 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. We also derive empirical estimates of the trade-offs and show their convergence to the corresponding population counterparts. Finally, we numerically quantify the trade-offs on representative problems and compare to the solutions achieved by baseline representation learning algorithms.

1 Introduction

Real-world applications of representation learning algorithms often have 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 underlying 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 pertaining to a desired semantic attribute \( S \) (e.g., age, gender or race). When \( Y \) is independent of \( S \), one can learn a representation that is independent of \( S \) with no loss of performance, i.e., no trade-off exists between the two objectives. However, when the two attributes \( Y \) and \( S \) are correlated, attaining semantic independence will necessarily reduce the performance of the target predictor, i.e., there is a trade-off between the two objectives. The trade-off is unknown yet is important for understanding the limits of existing and future representation learning algorithms that involve semantic independence constraints.

Let \( Z = f(X) \) be a representation of input data \( X \), and \( f(\cdot) \) be the encoder (see Fig 1(a)). Invariant learning requires that prediction of the target label, \( \hat{Y} = g_Y(Z) \) be independent of a semantic attribute \( S \) i.e., \( \hat{Y} \perp \perp S \) for all possible downstream target predictors \( g_Y(\cdot) \). This independence condition is satisfied if and only if (iff), the representation \( Z \) is independent of \( S \) i.e., \( Z \perp \perp S \). Therefore, Invariant...
representation learning (IRL) seeks to optimize two objectives: i) the degree of dependence between data representation $Z$ and semantic attribute $S$, and ii) target task utility. These two objectives can be combined into one, with a parameter $\tau$ controlling the trade-off.

In this paper, we identify and analytically determine two fundamental trade-offs in the invariant representation learning setting introduced above, namely Data Space Trade-Off and Label Space Trade-Off. These trade-offs are illustrated in Figures 1(b) and formally defined next.

**Definition 1.** Data Space Trade-Off arises from the statistical dependence between the target attribute $Y$ and the semantic attribute $S$ given the input data $X$. The data representation $Z$ is independent of the input data $X$, i.e. there exist no $f_{Y}()$ or $f_{S}()$ such that $Y = f_{Y}(X)$ or $S = f_{S}(X)$. When the learner’s hypothesis class contains all Borel-measurable functions, this trade-off is characterized as:

$$\inf_{f() \text{ measurable}} \left\{ (1 - \tau) \inf_{g_{Y}() \text{ measurable}} \mathbb{E}_{X,Y} \left[ \mathcal{L}_{Y} \left( g_{Y}(f(X)), Y \right) \right] + \tau \text{dep}(f(X), S) \right\} \quad (1)$$

where $f()$ is the encoder that extracts representation $Z$ from $X$, $g_{Y}()$ predicts $\hat{Y}$ from the representation $Z$, $\mathcal{L}_{Y}(\cdot, \cdot)$ is the loss for predicting the task label $Y$. The function $\text{dep}(\cdot, \cdot) \geq 0$ is a parametric or non-parametric measure of statistical dependence i.e., $\text{dep}(Q, U) = 0$ when $Q$ and $U$ are independent, and $\text{dep}(Q, U) > 0$ if $Q$ and $U$ are dependent with larger values indicating greater degrees of dependence. The scalar $\tau \in [0,1]$ is a hyper-parameter that controls the trade-off between the two objectives, with $\tau = 0$ being the standard representation learning that enforces no independence to the attribute $s$, while $\tau \rightarrow 1$ enforces representation $Z$ to be independent of $S$.

Including all measurable functions in the hypothesis class of the encoder $f()$ and target predictor $g_{Y}()$ 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 the mean-squared error, the optimal Bayes estimator, $g_{Y}(f(X)) = \mathbb{E}_{Y \mid X}$ is reachable. This definition corresponds to the trade-off $D$ in Figure 1(b).

**Definition 2.** Label Space Trade-Off arises by disregarding the imperfection of the input data $X$ for predicting the target feature $\hat{Y}$ or the semantic attribute $S$. In other words, this trade-off is purely

More specifically, we consider square-integrable Borel-measurable functions for boundedness.
We denote the trace of any square matrix $K$ as $\text{Tr}[K]$. Assumption 1. where $L$ is an ideal representation.

Contributions: i) Identify two fundamental trade-offs in invariant representation learning. ii) Obtain closed-form solution for the corresponding optimization problems, and consequently determine the trade-offs exactly. iii) Provide consistent empirical closed-form solution for the encoder that achieve optimal trade-offs. iv) Numerically quantify the trade-offs defined here and compare them to those obtained by existing solutions.

Implications: i) Our closed-form empirical estimators for the optimal representations lend themselves to practical invariant representation learning algorithms. ii) Theoretically elucidating and empirically quantifying the intrinsic limits of invariant representations will enable researchers and practitioners alike to identify the feasible and infeasible solution space for the trade-offs and lead to informed development and deployment of optimal IRL methods. iii) Our theoretical analysis sheds light on the utility-invariance trade-off, the role of statistical dependency between target label $Y$ and the semantic attribute $S$ given or regardless of the input data $X$.

2 Problem Setting

2.1 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 random vectors by regular upper case letters, e.g. $H$, $\Theta$ and the entry in $i$’s row, $j$’s column of any matrix $M$ is denoted by $(M)_{ij}$ or $m_{ij}$. Identity matrix of dimension $n \times n$ is denoted by $I_n$, or simply $I$ and a vector of ones with dimension $n \times 1$ is denoted by $1_n$ or $1$. We denote the trace of any square matrix $K$ by $\text{Tr}[K]$. Both finite and infinite sets are denoted by calligraphy letters, e.g. $\mathcal{H}$, $\mathcal{A}$.

2.2 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 random vector $(X, Y, S)$, 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 multidimensional regression target tasks where the semantic attribute can be either discrete or multidimensional continuous.

Assumption 1. We assume that the encoder consists of $r$ functions in an universal RKHS $(\mathcal{H}_X, k_X(\cdot, \cdot))$ (e.g., Gaussian kernel), where universality guarantees that $\mathcal{H}_X$ can approximate any Borel-measurable function with arbitrary precision $[5]$.

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

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

This is the case when the $\sigma$-algebra generated by $Y$ is not a subset of the $\sigma$-algebra generated by $X$. 

where $r$ is the dimensionality of the representation $Z$. As discussed in Corollary 4.1, unlike common practice where it is chosen arbitrarily, $r$ itself 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, $\inf_{g_Y} \mathbb{E}_{X,Y}[\mathcal{L}_Y(\alpha_Y(Z), Y)]$ in (1) with the negative of a non-parametric measure of dependence i.e., $-\text{dep}(Z, Y)$. We justify this substitution in the following:

The primary objective of this paper is representation learning that can be used for different downstream target tasks with different loss functions. Maximizing statistical dependency between the representation vector $Z$ and the target attribute $Y$ can flexibly learn a representation that is effective for different downstream target tasks, including, regression, classification, clustering, etc [6]. Particularly, in Section 3.5 we will show that with the appropriate tuning of dep$(Z, Y)$, our formulation specializes in learning a representation that is equivalent to Bayes predictor $\mathbb{E}_X[Y|X]$. Furthermore, in unsupervised settings, where there is no target attribute $Y$, the target dependence dep$(Z, Y)$ can be replaced with dep$(Z, X)$, which implicitly forces the representation $Z$ to retain as much information as is necessary for reconstructing the input data $X$. This scenario is of practical interest when a data producer aims to provide a representation of data that is independent of a desired semantic attribute for any arbitrary downstream task.

We start by designing dep$(Z, S)$, and dep$(Z, Y)$ follows similarly. A key desiderata of dependence measures is that they should be able to account for all possible non-linear dependence relations between the random variables (or vectors). Examples of such measures include information theoretic measures such as mutual information (e.g., MINE [7]). Calculating mutual information for high-dimensional continuous variables is computationally intractable and analytically challenging. Kernel methods for measuring of independence are an alternative solution with the attractive properties of being computationally feasible/efficient and analytically tractable. Kernel methods usually deploy covariance operator such as Hilbert-Schmidt Independence Criterion [8], Constrained Covariance [9] and Kernel Canonical Correlation [10]. The underlying principle behind the kernel method based dependence measures is that finite dimensional spaces with non-linear dependencies behave as linearly dependent spaces when mapped appropriately to higher dimensional spaces. In this paper we adopt the covariance operator based measures as our choice of dependence measure for analytical tractability.

Principally, $Z$ and $S$ are independent iff $\text{Cov}(\alpha(Z), \beta_S(S))$ is zero for all $\alpha(\cdot)$ and $\beta_S(\cdot)$ belonging to some universal RKHSs [9]. Since $Z = f(X)$ and $f(\cdot) \in \mathcal{H}_X$, $\text{Cov}(\alpha(Z), \beta_S(S)) = \text{Cov}(\alpha(f(X)), \beta_S(S))$, which necessitates application of a kernel on top of another kernel. This limits the analytical tractability of our solution. However, as we argue below, it is almost sufficient to consider transformation on $S$, only, in which case it reduces to $\text{Cov}(f(X), \beta_S(S))$. Let $(\mathcal{H}_S, k_S(\cdot, \cdot))$ and $(\mathcal{H}_Y, k_Y(\cdot, \cdot))$ be separable RKHSs of functions defined on $\mathbb{R}^{d_S}$ and $\mathbb{R}^{d_Y}$, respectively. Consider the bi-linear functional,

$$h(\cdot, \cdot): \mathcal{H}_X \times \mathcal{H}_S \to \mathbb{R}, h(f, \beta_S) := \text{Cov}_{X,S}(f(X), \beta_S(S)).$$

\textbf{Assumption 2.} We assume in the rest of this paper that the positive definite kernel functions are bounded, i.e.,

$$\mathbb{E}_X[k_X(X, X)] < \infty, \quad \mathbb{E}_S[k_X(S, S)] < \infty \quad \text{and} \quad \mathbb{E}_Y[k_Y(Y, Y)] < \infty.$$  

\textsuperscript{3}A Hilbert space is separable if it has a countable orthonormal basis set.
The assumptions in (5) guarantee that $h(\cdot, \cdot)$ in (4) is bounded [11] and therefore, invoking Riesz representation theorem [12], there exists a unique and bounded linear operator $\Sigma_{SX}$, such that
\[
h(f, \beta_s) = \text{Cov}_{X,S}(f(X), \beta_S(S)) = \langle \beta_S, \Sigma_{SX} f \rangle_{\mathcal{H}_S} \quad \forall f \in \mathcal{H}_X, \forall \beta_X \in \mathcal{H}_S.
\] (6)

Based on $h(\cdot, \cdot)$, we define the linear operator $h_{f,S} : \mathcal{H}_S \to \mathbb{R}^r$ as
\[
h_{f,S}(\beta_S) := \begin{bmatrix}
\text{Cov}_{X,S}(f_1(X), \beta_S(S)) \\
\vdots \\
\text{Cov}_{X,S}(f_r(X), \beta_S(S))
\end{bmatrix} = \begin{bmatrix}
\langle \beta_S, \Sigma_{SX} f_1 \rangle_{\mathcal{H}_S} \\
\vdots \\
\langle \beta_S, \Sigma_{SX} f_r \rangle_{\mathcal{H}_S}
\end{bmatrix}.
\]

The operator $h_{f,S}$ captures all modes of non-linear dependence, since the distribution of a low-dimensional projection of high-dimensional data is approximately normal [13], [14]. In other words, we assume that $(f(X), \beta_S(S))$ is an approximately normal random vector.

Among the different dependence measures that have been defined through the covariance operator we adopt a criterion similar (not exactly) to Hilbert-Schmidt Independence Criterion (HSIC) [8] which is defined as the Hilbert-Schmidt norm (HS-norm) of the covariance operator,
\[
\text{dep}(Z, S) := \| h_{f,S} \|^2_{HS} = \sum_{\beta_S \in \mathcal{U}_S} \| h_{f,S}(\beta_S) \|^2 = \sum_{\beta_S \in \mathcal{U}_S} \sum_{j=1}^r h^2(f_j, \beta_S)
\] (7)

where $\mathcal{U}_S$ is a countable orthonormal basis set for $\mathcal{H}_S$. Note that, HSIC carries an additional summation over an orthonormal basis set for $\mathcal{H}_X$, as well. Observe that based on this definition, if the distribution $(f(X), \beta_S(S))$ fails to be a normal distribution, we end up measuring mean dependency of $Z = f(X)$ from $S$ which is still much stronger than measuring the linear dependency between $Z$ and $S$ [15]. Even under this assumption, empirically (Section 5) we observe that trade-offs we obtain significantly dominate those from existing invariant representation learning algorithms.

A well-defined population expression for (7) is given in Section A. In the following we establish a procedure to empirically estimate $\text{dep}(Z, S)$ as well.

**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 from the joint distribution $p_{X,Y}$. Using, the representer theorem [16], 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 $(K_S)_{ij} = k_S(s_i, s_j)$. Let an empirical estimation of covariance be
\[
\text{Cov}_{X,S}(f_j(X), \beta_S(S)) \approx \frac{1}{n} \sum_{i=1}^n f_j(x_i) \beta_S(s_i) - \frac{1}{n^2} \sum_{i=1}^n \sum_{k=1}^n f_j(x_i) \beta_S(s_k).
\]

Then, the empirical estimator of $\text{dep}(Z, S)$ is given by
\[
\text{dep}^{\text{emp}}(Z, S) := \frac{1}{n^2} \| \Theta K_X H L_S \|^2_F,
\] (8)

where $H = I_n - \frac{1}{n} 1_n 1_n^T$ is centering matrix, and $L_S$ is a full row-rank matrix in which $L_S L_S^T = K_S$ (Cholesky factorization). This empirical estimator in [8] has a bias of $\mathcal{O}(n^{-1})$ and a convergence rate of $\mathcal{O}(n^{-1/2})$.

Similarly, we can define the dependence measure between $Z$ and $Y$ and its empirical version, i.e. $\text{dep}(Z, Y)$ and $\text{dep}^{\text{emp}}(Z, Y)$.
3 Fundamental Trade-Offs

3.1 Trade-Off D

We now turn to the the optimization problem corresponding to the trade-off $D$ in (1). Recall that $Z = f(X)$ is an $r \times 1$ random vector, where the dimensionality $r$ is a free variable. A common desiderata of learned representations is that of compactness [17] 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 $L_2$–universal RKHS $\mathcal{H}_X$, we impose additional constraints on the representation. Specifically, we constrain the search space of the encoder $f(\cdot)$ to learn a disentangled representation [17] as follows,

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

where $\gamma > 0$ a regularization parameter. The $\text{Cov}_X(f_i(X), f_j(X))$ part enforces the covariance of $Z$ to be identity matrix. This kind of disentanglement is used in PCA and, it enables us to ensure that the variance of each entry of $Z$ is bounded and different entries of $Z$ are uncorrelated to each other. The regularization part, $\gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}$ encourages the encoder components to be as orthogonal as possible to each other and to be of unit norm. This part helps with numerical stability during empirical estimation [11]. In Section 5, we suggest that $\gamma$ can be tuned through cross-validation. Furthermore, in the following Theorem, we show that 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 $A_r$.

This Theorem implies that disentanglement preserves the performance of downstream target task since the target predictor can revert the disentanglement $t$ and reach out to the original representation $Z$. Additionally, any measurable transformation of $Z$ will not add any more information about $S$ compared to the information that $Z$ already entails about $S$.

Now, the optimization problem in (1) reduces to,

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

where as justified earlier the target loss function $\inf_{f_X} E_{X,Y}[\mathcal{L}_Y(f_T(f(X)), Y)]$ is substituted by $-\text{dep}(f(X), Y)$. Fortunately, the above optimization problem lends itself to a closed-form solution as given by the next theorem.

**Theorem 3.** A solution to the optimization problem in (10) is the eigenfunctions corresponding to $r$ largest eigenvalues of the following generalized problem

$$\left( (1 - \tau) \Sigma^*_Y \Sigma_X - \tau \Sigma^*_X \Sigma_{XS} \right) f = \lambda (\Sigma_{XX} + \gamma I_r) f,$$

where $\Sigma_{XX}$ and $\Sigma_{XS}$ are the covariance operators defined in (6), and $\Sigma^*_X$ and $\Sigma^*_S$ are the adjoint operators of $\Sigma_{XX}$ and $\Sigma_{YS}$, respectively.

**Remark.** If the trade-off parameter $\tau = 0$ (i.e. no semantic independence constraint is imposed), the solution in Theorem 3 is equivalent to supervised PCA if further $\gamma \rightarrow 0$. On the other hand, if $\tau \rightarrow 1$ (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 $\Sigma^*_X \Sigma_{XS}$, which are the directions that are least explanatory of the semantic attribute $S$.

Now, consider the empirical version of (10):

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

where $\text{dep}^{\text{emp}}(f(X), S)$ and $\text{dep}^{\text{emp}}(f(X), Y)$ are given in (8).

\footnote{The term 'solution' in any optimization problem in this paper refers to a global optima.}
Theorem 4. Let the Cholesky factorization be \( K_X = L_X L_X^T \), where \( L_X \) is a full row-rank matrix. A solution to (12) is

\[
\mathbf{f}^{\text{opt}} = \Theta^{\text{opt}} \left[ k_X(\mathbf{x}_1, \cdot), \ldots, k_X(\mathbf{x}_n, \cdot) \right]^T
\]

where \( \Theta^{\text{opt}} = U^T (L_X)^\dagger \) and the columns of \( U \) are eigenvectors corresponding to \( r \) largest eigenvalues, \( \lambda_1, \ldots, \lambda_r \) of the following generalized problem,

\[
\left( L_X^T ((1 - \tau) \mathbf{K}_Y - \tau \mathbf{K}_S) L_X \right) \mathbf{u} = \lambda \left( \frac{1}{n} \mathbf{L}_X^T \mathbf{H} \mathbf{L}_X + \gamma I \right) \mathbf{u}
\]

where \( \gamma \) is the disentanglement regularization parameter defined in (9) and the supremum value of (12) is \( \sum_{j=1}^{r} \lambda_j \).

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

\[
\arg \sup_r \left\{ \sup_{f \in A_r} \left\{ J^{\text{emp}}(f(X)) := (1 - \tau) \text{dep}^{\text{emp}}(f(X), Y) - \tau \text{dep}^{\text{emp}}(f(X), S) \right\} \right\}
\]

which is the number of positive eigenvalues of the generalized eigenvalue problem in (13).

To intuitively 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. More discussion can be found in the supplementary material.

In the following Theorem, we prove that the empirical solution converges to its population counterpart.

Theorem 5. Assume that \( k_x(\cdot, \cdot) \) and \( k_y(\cdot, \cdot) \) are bounded by one and \( f_k^2(\mathbf{x}_i) \) is bounded by \( M \) for any \( k = 1, \ldots, r \) 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

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

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

3.2 Bayesian Optimality of Trade-Off D

In this Section we show that maximizing \( \text{dep}(f(X), Y) \) can learn a representation \( Z \) that is reach enough to lend itself to the optimal Bayes prediction of \( Y \) given the input data \( X \).

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 equation (11). Then, there exist a linear regression on top of the representation \( Z = f^*(X) \) that is equivalent to the Bayes regressor \( \mathbb{E}_Y[Y|X] \), i.e.

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

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

3.3 Trade-Off L

Following Section 2.2 we deploy \( -\text{dep}(Z, Y) \), defined similar to \( \text{dep}(Z, S) \) in (7), as a proxy for the loss function \( \inf_{g_Y \in \mathcal{H}_Y} \mathbb{E}_{X,Y} \left[ L_T(g_T(Z), Y) \right] \). We recall that label space trade-off arises when the representation \( Z \) is ideal and it does not need to be a function of \( X \). We can formulate the trade-off \( L \) as

\(\)
\[
\sup_{Z \in L^2} \left\{ J(Z) := (1 - \tau) \text{dep}(Z, Y) - \tau \text{dep}(Z, S) \right\},
\]
(15)

where \(L^2\) is the space of all random vectors of dimension \(r\) with finite variance, i.e., \(\mathbb{E}_Z \|Z - \mathbb{E}[Z]\|^2 < \infty\). Observe from (15) that the optimal \(Z\) is a function of \(p_{Y,S}\). Therefore, optimal \(Z\) is in the form of

\[
Z = f_L(Y, S)
\]
(16)

where \(f_L(\cdot, \cdot) : \mathbb{R}^d_y \times \mathbb{R}^d_s \rightarrow \mathbb{R}^r\) is a Borel-measurable function. Instead of directly optimizing over \(Z \in L^2\), equivalently, we optimize over all Borel-measurable functions \(f_L(\cdot, \cdot)\):

\[
\sup_{f_L \in \mathcal{A}_r(Y,S)} \left\{ (1 - \tau) \text{dep}(f_L(Y, S), ) - \tau \text{dep}(f_L(Y, S), S) \right\},
\]
(17)

where \(\mathcal{A}_r(Y,S)\) is defined similar to \(\mathcal{A}_r\) in (9) and replacing \(X\) by \((Y, S)\). Recall that \(\mathcal{A}_r(Y,S)\) ensures that \(Z\) will not contain highly correlated (entangled) dimensions, and thus be minimally redundant or maximally compact without degrading the performance of downstream target task.

**Remark.** The optimization problem in (17) and its empirical counterpart can be solved similar to that of trade-off \(D\) in Theorems 3 and 4 where \(X\) is replaced by \((Y, S)\).

### 3.4 Trade-Off \(L\) vs Trade-Off \(D\)

Let \(\sigma(X)\) be the \(\sigma\)-algebra generated by the random vector \(X\). If we assume that \(Z = f(X)\), then the \(\sigma\)-Algebra generated by \(Z\) (i.e., \(\sigma(Z)\)) is always a subset of \(\sigma(X)\). In Trade-Off \(L\), the random vector \(Z\) is not a function of \(X\) which means that \(\sigma(Z)\) is not necessarily a subset of \(\sigma(X)\). Therefore, for an ideal \(Z\) in trade-off \(L\), there may not exist a valid encoder that can map \(\sigma(X)\) to \(\sigma(Z)\). For example, let the ideal embedding \(Z\) be equal to \(X + U\), where \(U\) is a random vector independent of \(X\). In this setting there is no measurable function \(f\) which can relate \(Z\) as a function of \(X\) since \(\sigma(Z) \not\subseteq \sigma(X)\).

To see the effect of this analysis intuitively, assume that \(X\) does not provide sufficient information about the target attribute \(Y\) to perfectly predict it. In this case there will be neither a perfect predictor nor a perfect representation from \(X\) to describe \(Y\). However, if we do not limit our representation \(Z\) to be a function of \(X\), we can set \(Z\) to be equal to \(Y\). For the case of invariant representation learning, this idealization of \(Z\) is useful as an upper bound on the best possible trade-off achievable by any learning algorithm. We reaffirm that there will be a non-zero gap between trade-off \(L\) and data trade-off \(D\) if data does not contain sufficient information to perfectly predict the target and semantic attributes.

### 3.5 Trade-Off \(F\)

Here we define and discuss the trade-off achievable by practical realizations of representation learning algorithms with either fairness, invariance or semantic independence constraints.

**Definition 4.** **Feasible Space Trade-Off** arises from the statistical dependence between the target feature \(Y\) and the sensitive attribute \(S\) conditioned on the given input data \(X\), the choice of hypothesis class for the learners involved, and the choice of dependence measure adopted. This setting can be formalized as,

\[
\inf_{g_Y \in \mathcal{H}_Y} \inf_{f \in \mathcal{H}_X} \left\{ (1 - \tau) \mathbb{E}_{X,Y} \left[ \mathcal{L}_Y(g_Y(f(X)), Y) \right] + \tau \text{dep}(f(X), S) \right\}, \quad 0 \leq \tau < 1,
\]
(18)

where \(\mathcal{H}_X\) and \(\mathcal{H}_Y\) are the hypothesis class for the encoder network and target predictor, respectively, \(\mathcal{L}_Y(\cdot, \cdot)\) denotes the loss function of target task, and \(\text{dep}(f(X), S)\) is a parametric or non-parametric surrogate measure of dependency quantifying the dependency between representation vector \(Z = f(X)\) and the sensitive attribute \(S\).

This setting corresponds to the trade-off \(F\) in Figure 1(b), and is necessarily dominated by the Data Space Trade-Off \(D\). Multiple factors may lead to such sub-optimal trade-offs. These include, hypothesis classes of target and/or encoder are not containing all measurable functions (e.g., [18] considers...
non-universal neural networks for encoder), the surrogate dependence measure \( \widetilde{\text{dep}}(f(X), S) \) does
not account for all non-linear dependencies (e.g., \([3,2,19,4]\) which consider adversarially learned
dependence measures), sub-optimal optimization of \( (18) \) in terms of achieving only local optima but
not the global optima (e.g., when the hypothesis class is deep neural networks that are optimized
through stochastic gradient descent, or through stochastic gradient descent-ascent in the case of
adversarial representation learning\([3,19,2]\), and combinations thereof.

4 Related Works

4.1 Invariant, Fair, Privacy-Preserving Representation Learning

The basic idea of representation learning that discards unwanted semantic information has been
explored under different contexts like invariant, fair, or privacy-preserving learning. In domain
adaptation\([20,21,22]\), the goal is to learn features that are independent of the data domain. In fair
learning\([23,24,25,26,27,28,29,19,30,31,2,32,33,34,35,36,4]\), the goal is to discard the
demographic information that leads to unfair outcomes. Similarly, there is a growing interest in
mitigating unintended leakage of private information from data representations\([37,38,1,39,40]\). A
vast majority of this body of work is empirical in nature. These methods implicitly look for a single
or more points in the trade-off between utility and fairness and do not explicitly seek to characterize
the whole trade-off front. Overall, these approaches are not concerned (or aware) about the feasibility
and limitations on the utility-invariance trade-off. In contrast, this paper determines the fundamental
theoretical limits of controlling independence to semantic attributes, and proposes practical learning
algorithms that achieve this limit.

4.2 Adversarial Representation Learning

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

\[
\inf_{f \in \mathcal{H}_f} \left\{ (1 - \tau) \inf_{g_y \in \mathcal{H}_y} \mathbb{E}_{X,Y} \left[ \mathcal{L}_Y(g_y(f(X)), Y) \right] - \tau \inf_{g_S \in \mathcal{H}_s} \mathbb{E}_{X,S} \left[ \mathcal{L}_S\left(g_S(f(X)), S\right) \right] \right\}, \tag{19}
\]

where \( \mathcal{L}_S(\cdot, \cdot) \) is the loss function of a hypothetical adversary \( g_S(\cdot) \) 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 \([4]\) where the negative loss of the adversary, 

\[
- \inf_{g_S \in \mathcal{H}_s} \mathbb{E}_{X,S} \left[ \mathcal{L}_S\left(g_S(f(X)), S\right) \right]
\]

does the role of \( \text{dep}(f(X), S) \). However, this form of adversarial learning suffers from a drawback
that the induced measure of dependence does not account for all modes of non-linear dependence
between \( S \) and the representation \( Z \) if the loss function \( \mathcal{L}_S \) is mean-squared error (MSE) or cross-
entropy\([41,42]\). This implies that an optimal adversary does not necessarily lead to a representation
\( Z \) that is statistically independent of \( S \), i.e., \( p(S \mid Z) = p(S) \). Therefore, the adversary loss in ARL
should be carefully designed to account for all modes of dependence between \( Z \) and \( S \).

4.3 Trade-Offs in Invariant Representation Learning:

In this Section, we compare our work, based on several important properties, with the previous works
that aim to characterize utility-invariance trade-offs.

**Restricted Class of Attributes:** Most related works are restricted to binary and/or categorical \( Y \) and
\( S \). For instance, \([43]\) 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 \([44]\) provided both upper and lower
bound for the binary labels. By leveraging Chernoff bound, \([45]\) 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 \([46]\). In contrast to this body of works, 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 \([4] \) and \([47]\). However, in \([47]\), 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:** It is common among existing works to measure the dependence between the representation $Z$ and the semantic attribute $S$ via an adversary optimizing an MSE or cross-entropy loss. Such dependence measures cannot capture all modes of statistical dependency if $S$ is not binary (see [41] for more details). Some examples deploying MSE/cross entropy loss in adversarial setting are [46], [47], and [4]. In contrast, our formulation is capable of capturing all modes of dependency through some universal RKHSs. To give some intuition why MSE loss cannot account for all modes of dependency, we consider the most closely related work [47]. In this paper, an upper bound for the utility-invariance trade-off is found in terms of the top two eigenvectors of $\Sigma_{XX}^{1/2}(\tau aa^T - yy^T)\Sigma_{XX}^{1/2}$, where $a$ and $b$ are optimal Bayes regressors for $S$ and $Y$, respectively. However, the $\Sigma_{XX}^{1/2}(\tau aa^T)\Sigma_{XX}^{1/2}$ part, that is supposed to capturing the statistical dependency between $S$ and the representation $Z$, is restricted to only looking for mean independence rather than all modes of dependency. In classification, the aim of any adversary is to maximize the probability of predicting the true class. Therefore, any representation $Z$ that imposes the Bayes classifier on $Z$ to assign equal probabilities to each class in $S$ is an optimal representation. But, this optimal representation does not necessarily imply independence between $Z$ and $S$. In contrast, our characterization in (11) is looking at all possible kinds of dependency via $\Sigma_{SX}\Sigma_{SX}$ and it is not restricted by any adversary task.

**Characterizing Trade-Off:** To the best of our knowledge, all exciting approaches except [4] characterize the trade-off in terms of some bounds (upper and/or lower). In contrast, we are able to characterize both data space and label space trade-offs in an exact closed-form expression where unlike [4] our trade-off is not sub-optimal.

**Optimal Encoder** Compared to the related works with the general class of attributes, this paper is the only work that is providing computationally tractable learning algorithms for optimal encoders that achieve the exact trade-offs (see Theorem [4] and Corollary [4.1]). Even though [4] is also providing a representation learning algorithm, however, this algorithm is not induced by an optimal trade-off characterization due to restriction to only linear dependency between $Z$ and $S$.

### 5 Numerical Estimation of Trade-Offs

In this section, we demonstrate the practical utility of the analytical results developed in the paper and validate our theoretical insights.

#### 5.1 Gaussian Mixture

In the first experiment, we design an illustrative toy example that conforms to the setting studied in the paper and numerically quantify the trade-offs that we introduced.

Consider the following Gaussian mixture model from which we generate 4000, 2000, and 2000

$$V = [V_1, V_2] \sim \frac{1}{2} \left( \mathcal{N}(m, \Sigma) + \mathcal{N}(m', \Sigma) \right), \quad m = [0, 1], \ m' = [1, 1], \ \Sigma = \text{diag}(0.1^2, 0.1^2)$$

independent samples for training, validation and testing, respectively. Figure [3]a) shows the test samples where the samples generated with $m$ and $m'$ are in blue and red, respectively. The input data $X$ is set to $V_1$ (the first entry of $V$), the sensitive attribute $S$ is $V_3^3$, and the target attribute $Y$ is $[V_1, V_3^3]$. Therefore, both input data and target attributes are dependent on the sensitive attribute.

**Trade-Offs D & L:** The optimal $Z$ is learned for the trade-off $D$ through the closed-form solution in Theorem [4] for different invariance parameter values $\tau$ in $[0, 1]$. Then, this optimal embedding is fed to a target task predictor which is a multi-layer perceptron (MLP) with two hidden layers, and 4, 8 neurons where we use MSE as a loss function and AdamW [48] as an optimizer. The x-axis is a normalized version of the dependence measure used in our optimization, while the y-axis quantifies utility normalized to $[0, 1]$ as $\exp(-\text{MSE})$. The same procedure is implemented for trade-off $L$, except that the input data is $V$, instead of $X$. These trade-offs are shown in Figure [3]b). The reason that we choose the input data to be $V$ instead of $(Y, S)$ for trade-off $L$ is that $(Y, S)$ is fully generated from $V$. For $\tau = 0$ and $\tau = 0.5$, the optimal embeddings are illustrated in Figure [3]c) and (d), respectively. Since the sensitive attribute is only related to $V_1$, an invariant embedding should collapse the corresponding dimension and cause the two colors to overlap with each other. We choose the number of epochs and batch-size to be 500 and optimize the learning rate by trying six different values among $\{10^{-2}, 10^{-3}, 3 \times 10^{-4}, 5 \times 10^{-4}, 10^{-3}, 10^{-5}\}$. We consider Gaussian kernel for all $\mathcal{H}_X$. 

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Figure 3: (a): A mixture of two Gaussians that generates the input data as $X = V_1$, the sensitive attribute as $S = V_3^Z$, and the target attribute as $Y = [V_1, V_3^Y]$. (b): Two fundamental trade-offs, $D$ and $L$, together with two baseline trade-offs $F$, ARL optimized with SGDA [19] and global optima of ARL with a linear RKHS [4]. (c), (d): The learned embedding for $\tau = 0$ and $\tau = 0.5$, respectively. An invariant representation should collapse $V_1$, i.e., the two colors should fully overlap with each other in the embedding. The overlap is partial for $\tau = 0.5$ and as $\tau \to 1$, the optimal representation is zero.

$H_S$ and $H_Y$ and seek the band-width (i.e., $\sigma$) of Gaussian kernels using five different logarithmically spaced values in $[10^{-2}, 10^2]$. Further, we optimize the regularization parameter $\gamma$ in equation (10) by considering three values among $\{0, 10^{-4}, 1\}$. We first set $\sigma_X = \sigma_S = \sigma_Y = 1, \gamma = 10^{-4}$ and explore the optimal learning rate by minimizing MSE in the validation set. Once the learning rate is found, we explore $\sigma$’s by minimizing MSE on the validation set. In the end, we explore $\gamma$ similarly.

Spectral Adversarial Representation Learning (Spectral-ARL): Spectral ARL [4] is very similar to the trade-off $D$ of this paper except that $H_S$ and $H_Y$ are both linear RKHS. We followed the same experimental setting of trade-off $D$. The results of this approach are illustrated in Figure 3 (c).

Adversarial Representation Learning (ARL): We followed the ARL formulation in (3) for different invariance parameter values $\tau$ in $[0, 1)$. The embedding $Z = f(X)$ is extracted via the encoder $f(\cdot)$ which is an MLP with two hidden layers, and 4, 2 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 4, 8 neurons. We use stochastic gradient descent-ascent (SGDA) [19] with AdamW [48] 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 500 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 by. Since ARL can be unstable, we run our experiment for five different random seeds. The mean and standard-deviation (std) of the results are illustrated in Figure 3.

We make the following observations, (a) Trade-off $L$ dominates trade-off $D$ as expected. (b) The trade-offs $F$ obtained by the baselines are dominated by trade-off $D$. Adversarial representation learning [3, 19, 2] uses sub-optimal optimization (SGDA), while Spectral-ARL [4] uses a global
optimum solution but restricts the hypothesis class in \[ (19) \] to linear RKHS. As such, the baselines are unable to match the global optimal solution of \[ (12) \], and (c) At \( \tau = 0.5 \) the embedding does indeed collapse \( V_1 \) to an extent leading to partial overlap between the two mixtures.

5.2 Fair Classification

In this experiment we consider a fair classification application of IRL on Adult dataset\(^5\). This dataset contains 45,222 instances of different individual where each instance includes 14 attributes. The target task is a binary classification of annual income (more or less than 50K) while the sensitive attribute (i.e., semantic attribute) in which we aim to be independent of it is \( S = \text{(race, gender)} \). We randomly split the data into training (25,222 instances), validation (10,000 instances), and testing (10,000 instances) and perform our experiment five times (each time with a different random seed on data split and weight initialization of involved networks).

We consider demographic parity (DP)\(^4\) as a fairness criterion, where the goal is to have the prediction of target feature \( \hat{Y} \) be independent of the sensitive feature \( S \). In the context of representation learning, DP exactly falls into IRL since \( \hat{Y} = g_Y(Z) \) is required by DP to be independent of \( S \) regardless of the target predictor \( g_Y(\cdot) \). Similar to\(^5\), we define DP violation (DPV) as

\[
\text{DPV} = \max_{S_0, S'_0} \left| \mathbb{P}[\hat{Y} | S = S_0] - \mathbb{P}[\hat{Y} | S = S'_0] \right|.
\] (20)

Following Section 5.1, we learn the optimal embedding \( Z \) for the trade-offs \( D \) and \( L \) using Theorem 4 for different invariance parameter values \( \tau \in [0, 1] \) and then feed this representation to a three-layer MLP with 64, 128, and 64 neurons, respectively. Similar RKHSs together with optimization procedure (except that the batch-size is 250) and hyperparameter tuning as Section 5.1 is deployed. The mean of results are illustrated in Figure 4. Note that the baseline method, spectral-ARL \(^4\) is almost similar to trade-off \( D \) where linear RKHS is used for both \( \mathcal{H}_S \) and \( \mathcal{H}_Y \). The mean of result is illustrated in Figures 4. For ARL method, the encoder \( f(\cdot) \) is a three-layer MLP with 64, 128 and 64 neurons, respectively. Both the target task predictor \( g_Y(\cdot) \) and proxy adversary \( g_S(\cdot) \) are MLP with the similar architectures to the encoder. We followed the same optimization procedure and hyperparameter tuning as Section 5.1 except that the batch-size is 250. The mean of ARL result is illustrated in Figures 4.

We observe that i) As expected, trade-off \( L \) dominates trade-off \( D \). ii) The two baseline methods (trade-offs \( F \)) are dominated by trade-off \( D \) which is due to the suboptimality of their optimization and dependence measures.

![Figure 4: Fair classification: Two fundamental trade-offs, \( L \) and \( D \), together with two baseline trade-offs \( F \), ARL optimized with SGDA \(^19\) and Spectral-ARL with a linear RKHS \(^4\).](#)

\(^{5}\)The data is downloaded from the UCI ML-repository at https://archive.ics.uci.edu/ml/datasets/adult.
6 Conclusions

This paper developed the theoretical underpinnings for identifying and determining the fundamental trade-offs and limits of representation learning under competing objectives. These trade-offs include i) label space trade-off which is solely induced by the statistical relation between target task and semantic attribute; ii) data space trade-off which is due to the imperfection of input data to predict the target or semantic attributes and the statistical dependence between target and semantic attributes. Further, we found closed-from solutions for the global optima, both the population and empirical versions, for the underlying optimization problems, and thus quantify the trade-offs exactly. Our results shed light on the regions of the trade-off that are feasible or impossible to achieve by learning algorithms. Numerical results suggest that commonly used adversarial representation learning based techniques are unable to reach the optimal trade-offs.

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\[ \text{A Population Expression for Equation (7)} \]

A population expression for \( \text{dep}(Z, S) \) in (7) is given in the following.

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

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

\[ \text{Proof.} \] We first note that this population expression is inspired by HSIC \([8]\). In our case, \( \text{dep}(Z, S) \) is defined for a fixed \( f \) where HS-norm is carried only on \( \beta_S \), while HSIC considers HS-norm on both \( \beta_S \) and \( f \).

Using definition (8), we get

\[
\text{dep}(Z, S) = \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} h^2(f_j, \beta_S) \\
= \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} \langle \beta_S, \Sigma_{SX} f_j \rangle^2_{\mathcal{H}_S} \\
= \sum_{j=1}^{r} \sum_{\beta_S \in \mathcal{U}_S} \langle \beta_S, \Sigma_{SX} f_j \rangle^2_{\mathcal{H}_S} \\
\overset{(a)}{=} \sum_{j=1}^{r} \| \Sigma_{SX} f_j \|_{\mathcal{H}_S}^2 \\
= \sum_{j=1}^{r} \langle \Sigma_{SX} f_j, \Sigma_{SX} f_j \rangle_{\mathcal{H}_S} \\
\overset{(b)}{=} \sum_{j=1}^{r} \text{Cov}_{X, S} \left( f_j(X), \langle \Sigma_{SX} f_j \rangle(S) \right) \\
= \sum_{j=1}^{r} \text{Cov}_{X, S} \left( f_j(X), \langle k_S(\cdot, S), \Sigma_{SX} f_j \rangle_{\mathcal{H}_S} \right) \\
= \sum_{j=1}^{r} \text{Cov}_{X, S} \left( f_j(X), \text{Cov}_{X', S'} \left( f_j(X'), k_S(S', S) \right) \right) \\
= \sum_{j=1}^{r} \text{Cov}_{X, S} \left( f_j(X), \mathbb{E}_{X', S'} [f_j(X') k_S(S, S')] - \mathbb{E}_X [f_j(X)] \mathbb{E}_{S'} [k_S(S, S')] \right) \\
= \sum_{j=1}^{r} \left\{ \mathbb{E}_{X, S, X', S'} \left[ f_j(X) f_j(X') k_S(S, S') \right] + \mathbb{E}_X [f_j(X)] \mathbb{E}_{X'} [f_j(X')] \mathbb{E}_{S, S'} [k_S(S, S')] \right. \\
\left. - 2 \mathbb{E}_X \left[ f_j(X) \mathbb{E}_{X'} [f_j(X')] \mathbb{E}_{S'} [k_S(S, S')] \right] \right\}
\]

where (a) is due to Parseval relation for orthonormal basis and (b) is from the definition of \( \Sigma_{SX} \) in (7). \( \square \)
B Proof of Lemma 1

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 $(K_S)_{ij} = k_S(s_i, s_j)$. Let an empirical estimation of covariance be

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

Then, the empirical estimator of $\text{dep}(Z, S)$ is given by

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

where $H = I_n - \frac{1}{n} 1_n 1_n^T$ is centering matrix, and $L_S$ is a full row-rank matrix in which $L_S L_S^T = K_S$ (Cholesky factorization). This empirical estimator in (8) 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

$$\langle \beta_i, \beta_m \rangle_{\mathcal{H}_S} = \left\langle \sum_{j=1}^n \alpha_j k_S(s_j, \cdot), \sum_{l=1}^n \eta_l k_S(s_l, \cdot) \right\rangle_{\mathcal{H}_S} = \sum_{j=1}^n \sum_{l=1}^n \alpha_j \eta_l k_T(y_j, y_l) = \alpha^T K_S \eta = \langle L_S^T \alpha, L_S^T \eta \rangle_{\mathcal{H}_S}$$

where $L_S \in \mathbb{R}^{n \times q}$ is a full row-rank matrix and $K_S = L_S L_S^T$ is the Chelesky factorization. As a result, $\beta_i \in U_S$ would become equivalent to $L_S^T \alpha \in U_q$ where $U_q$ is any complete orthonormal set for $\mathbb{R}^q$. Using empirical expression for covariance together with equations (7) and (8), we get

$$\text{dep}^{\text{emp}}(Z, S) := \sum_{\beta_j \in U_q} \sum_{j=1}^r \left\{ \frac{1}{n} \sum_{i=1}^n f_j(x_i)\beta_S(s_i) - \frac{1}{n^2} \sum_{i=1}^n \sum_{k=1}^n f_j(x_i)\beta_S(s_k) \right\}^2$$

$$= \sum_{L_S^T \alpha \in U_q} \sum_{j=1}^r \left\{ \frac{1}{n} \theta_j^T K_X K_Y \alpha - \frac{1}{n^2} \theta_k^T K_X 1_n 1_n^T K_Y \alpha \right\}^2$$

$$= \sum_{L_S^T \alpha \in U_q} \sum_{j=1}^r \left\{ \frac{1}{n} \theta_j^T K_X H K_S \alpha \right\}^2$$

$$= \sum_{L_S^T \alpha \in U_q} \sum_{j=1}^r \left\{ \frac{1}{n} \theta_j^T K_X H L_S L_S^T \alpha \right\}^2$$

$$= \sum_{\zeta \in U_q} \sum_{j=1}^r \left\{ \frac{1}{n} \theta_j^T K_X H L_S \zeta \right\}^2$$

$$= \frac{1}{n^2} \| \Theta K_X H L_S \zeta \|_2^2$$

$$= \frac{1}{n^2} \| \Theta K_X H L_S \|_F^2,$$

where $f(X) = \Theta [k_X(x_1, X), \ldots, k_X(x_n, X)]^T$ and $\Theta := [\theta_1, \ldots, \theta_r]^T$. 

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We now show that the bias of $\text{dep}_{\text{II}}(Z, S)$ to estimate $\text{dep}(Z, S)$ in (8) is $O\left(\frac{1}{n}\right)$. To do this, we split $\text{dep}_{\text{II}}(Z, S)$ into three terms as

\begin{equation}
\frac{1}{n^2} \|\Theta K_X H L S\|_F^2 = \frac{1}{n^2} \text{Tr} \left\{ \Theta K_X H K_S H K_X \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 \Theta K_X K_S \right\} - \frac{2}{n^3} \text{Tr} \left\{ 1^T K_X \Theta^T \Theta K_X K_S 1 \right\} + \frac{1}{n^3} \text{Tr} \left\{ 1^T K_X \Theta^T \Theta K_X 11^T K_S 1 \right\}
\end{equation}

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

(I):

\begin{equation}
\mathbb{E} \left[ \text{Tr} \left\{ K_X \Theta^T \Theta 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)_{ji} \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] = 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]
\end{equation}

where $(X, S)$ and $(X', S')$ are independently drawn from the joint distribution $p_{X,S}$.

(II):

\begin{equation}
\mathbb{E} \left[ 1^T K_X \Theta^T \Theta 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] = \sum_{k=1}^r \mathbb{E} \left[ \sum_i (\alpha_k \alpha_k^T)_{ii}(K_S)_{ii} + \sum_{(m,j) \in c^n_2} (\alpha_k \alpha_k^T)_{mn}(K_S)_{mj} \right] + \sum_{k=1}^r \mathbb{E} \left[ \sum_{(m,i) \in c^n_2} (\alpha_k \alpha_k^T)_{mi}(K_S)_{mi} + \sum_{(m,j) \in c^n_2} (\alpha_k \alpha_k^T)_{mj}(K_S)_{mj} \right]
\end{equation}

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Let \( \alpha \) Using above calculations together with Lemma 2 lead to

\[
\mathbb{E}\left[ \sum_{k=1}^{r} \mathbb{E}\left[ \sum_{(i,j) \in e_k^n} (\alpha_k \alpha_k^T)_{mi} (K_S)_{mj} \right] \right] \\
= n \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k^2(X)k_S(S,S) \right] + \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,S'} \left[ f_k^2(X)k_S(S,S') \right] \\
+ \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X'} \left[ f_k(X)f_k(X')k_S(S,S') \right] \\
+ \frac{n!}{(n-2)!} \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'} \left[ f_k(X)f_k(X')k_S(S,S') \right] \\
+ \frac{n!}{(n-3)!} \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k(X)\mathbb{E}_{X'}[f_k(X')][E_{S'}[k_S(S,S')]] \right]
\]

Using above calculations together with Lemma 2 lead to

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

We now obtain the convergence of \( \text{dep}_{\text{emp}}(Z,S) \). Consider the decomposition in (22) together with (23), (24), and (25). Let \( \alpha_k := K_X \theta_k \), then it follows that

\[
P\left\{ \text{dep}(Z,S) - \text{dep}_{\text{emp}}(Z,S) \geq t \right\} \\
\leq \sum_{k=1}^{r} \mathbb{E}_{X,S,X',S'} \left[ f_k(X)f_k(X')k_S(S,S') \right] - \frac{(n-2)!}{n!} \sum_{k=1}^{r} \sum_{(i,j) \in e_k^n} (\alpha_k \alpha_k^T)_{ij} (K_S)_{ji} + \mathcal{O}\left( \frac{1}{n} \right) \geq at \\
+ \sum_{k=1}^{r} \mathbb{E}_{X,S} \left[ f_k(X)\mathbb{E}_{X'}[f_k(X')][E_{S'}[k_S(S,S')]] \right] \\
\quad - \frac{(n-3)!}{n!} \sum_{k=1}^{r} \sum_{(i,j,m,l) \in e_k^n} (\alpha_k \alpha_k^T)_{mi} (K_S)_{mj} + \mathcal{O}\left( \frac{1}{n} \right) \geq bt \\
+ \sum_{k=1}^{r} \mathbb{E}_{X}[f_k(X)\mathbb{E}_{X'}[f_k(X')][E_{S,S'}[k_S(S,S')]]
\]
where $\gamma > k$ where we assumed that $a, b > 0$ 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 [51]

\[
u_1(\zeta_i, \zeta_j) = \frac{(n-2)!}{n!} \sum_{(i,j) \in c^n_i} \sum_{k=1}^r (\alpha_k \alpha_k^T)_{ij}(K_S)_{ij}
\]

\[
u_2(\zeta_i, \zeta_j, \zeta_m) = \frac{(n-3)!}{n!} \sum_{(i,j,m) \in c^n_i} \sum_{k=1}^r (\alpha_k \alpha_k^T)_{mj}(K_S)_{mj}
\]

\[
u_3(\zeta_i, \zeta_j, \zeta_m, \zeta_l) = \frac{(n-4)!}{n!} \sum_{(i,j,m,l) \in c^n_i} \sum_{k=1}^r (\alpha_k \alpha_k^T)_{lj}(K_S)_{ml}
\]

Then, from Hoeffding’s inequality [51] it follows that

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

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

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

Consequently, we have

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

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

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

(26)

**C 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 $\mathcal{A}_r$.

**Proof.** Recall that the space of disentangled representation is

\[
\mathcal{A}_r := \left\{ (f_1, \cdots, f_r) \left| f_i, f_j \in \mathcal{H}_X, \text{Cov}_X(f_i(X), f_j(X)) + \gamma(f_i, f_j) \mathcal{H}_X = \delta_{i,j} \right. \right\},
\]

where $\gamma \geq 0$. 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

\[
G_0 = \begin{bmatrix}
\langle f_1, f_1 \rangle_{\mathcal{H}_X} & \cdots & \langle f_1, f_r \rangle_{\mathcal{H}_X} \\
\vdots & \ddots & \vdots \\
\langle f_r, f_1 \rangle_{\mathcal{H}_X} & \cdots & \langle f_r, f_r \rangle_{\mathcal{H}_X}
\end{bmatrix}
\]

\[
G = G_0^{-1/2}
\]

\[
t_j \circ f = \sum_{m=1}^r g_{j,m}(\Sigma_{XX} + \gamma I_X)^{-1/2} f_j, \quad \forall j = 1, \cdots, r
\]
is the desired invertible transformation. To see this, construct

\[
\text{Cov}_X(t_i(f(X)), t_j(f(X))) + \gamma \langle t_i \circ f, t_j \circ f \rangle_{H_X}
\]

\[
= \langle t_i \circ f, (\Sigma_{XX} + \gamma I_X) t_j \circ f \rangle_{H_X}
\]

\[
= \left\langle \sum_{m=1}^{r} g_{i,m}(\Sigma_{XX} + \gamma I_X)^{-1/2} f_i, \sum_{k=1}^{r} g_{j,k}(\Sigma_{XX} + \gamma I_X)(\Sigma_{XX} + \gamma I_X)^{-1/2} f_j \right\rangle_{H_X}
\]

\[
= \sum_{m=1}^{r} \sum_{k=1}^{r} g_{i,m} g_{j,k} \langle f_i, f_j \rangle_{H_X} = \delta_{i,j}
\]

The inverse of \(t\) is \(t' = [t'_1, \ldots, t'_r]\) where

\[
H = G_0^{1/2}
\]

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

\[
\square
\]

D Proof of Theorem 3

**Theorem 3.** A solution to the optimization problem in (10) is the eigenfunctions corresponding to \(r\) largest eigenvalues of the following generalized problem

\[
\left( (1 - \tau) \Sigma_{YX} - \tau \Sigma_{SX}^* \Sigma_{XS} \right) f = \lambda (\Sigma_{XX} + \gamma I)f,
\]

where \(\Sigma_{SX}\) and \(\Sigma_{YX}\) are the covariance operators defined in (6), and \(\Sigma_{SX}^*\) and \(\Sigma_{YX}^*\) are the adjoint operators of \(\Sigma_{SX}\) and \(\Sigma_{YX}\), respectively.

**Proof.** Consider \(\text{dep}(Z, S)\) in (8):

\[
\text{dep}(Z, S) = \sum_{\beta_S \in U_S} \sum_{j=1}^{r} h^2(f_j, \beta_S)
\]

\[
= \sum_{j=1}^{r} \sum_{\beta_S \in U_S} \langle \beta_S, \Sigma_{SX} f_j \rangle_{H_S}^2
\]

\[
= \sum_{j=1}^{r} \| \Sigma_{SX} f_j \|_{H_S}^2,
\]

where the last step is due to Parseval’s identity for orthonormal basis. Similarly, we have \(\text{dep}(Z, Y) = \sum_{j=1}^{r} \| \Sigma_{YX} f_j \|_{H_Y}^2\).

Recall that \(Z = f(X) = (f_1(X), \cdots, f_r(X))\), then, it follows that

\[
J(f(X)) = (1 - \tau) \sum_{j=1}^{r} \| \Sigma_{YX} f_j \|_{H_Y}^2 - \tau \sum_{j=1}^{r} \| \Sigma_{SX} f_j \|_{H_S}^2
\]

\[
= (1 - \tau) \sum_{j=1}^{r} \langle \Sigma_{YX} f_j, \Sigma_{YX} f_j \rangle_{H_Y} - \tau \sum_{j=1}^{r} \langle \Sigma_{SX} f_j, \Sigma_{SX} f_j \rangle_{H_S}
\]

\[
= \sum_{j=1}^{r} \langle f_j, ((1 - \tau) \Sigma_{YX}^* \Sigma_{YX} - \tau \Sigma_{SX}^* \Sigma_{SX}) f_j \rangle_{H_X}
\]

where \(\Sigma^*\) is the adjoint operator of \(\Sigma\). Further, note that \(\text{Cov}_X(f_i(X), f_j(X))\) is equal to \(\langle f_i, \Sigma_{XX} f_j \rangle_{H_X}\). As a result, the optimization problem in (11) can be restated as

\[
\sup_{(f_i, (\Sigma_{XX} + \gamma I_X) f_k)_{H_X} = \delta_{i,k}} \sum_{j=1}^{r} \langle f_j, ((1 - \tau) \Sigma_{YX}^* \Sigma_{YX} - \tau \Sigma_{SX}^* \Sigma_{SX}) f_j \rangle_{H_X}, \quad 1 \leq i, k \leq r
\]
where \( I_X \) denotes identity operator from \( \mathcal{H}_X \) to \( \mathcal{H}_X \). This optimization problem is known as generalized Rayleigh quotient \( [52] \) and a possible solution to it is given by the eigenfunctions corresponding to the \( r \) largest eigenvalues of the following generalized problem
\[
(1 - \tau)\Sigma_{XY}\Sigma_{YX} - \tau \Sigma_{XS}\Sigma_{SX} \right) f = \lambda \left( \Sigma_{XX} + \gamma I_X \right) f.
\]

\[\square\]

E Proofs of Theorem 4 and Corollary 4.1

**Theorem 4.** Let the Cholesky factorization be \( K_X = L_X L_X^T \), where \( L_X \) is a full row-rank matrix. A solution to (12) is
\[
f^\text{opt} = \Theta^\text{opt}\left[ k_X(x_1, \cdot), \ldots, k_X(x_n, \cdot) \right]^T
\]
where \( \Theta^\text{opt} = U^T(L_X)^\dagger \) and the columns of \( U \) are eigenvectors corresponding to \( r \) largest eigenvalues, \( \lambda_1, \ldots, \lambda_r \) of the following generalized problem,
\[
\left( L_X^\dagger((1 - \tau)K_Y - \tau K_X) L_X \right) u = \lambda \left( \frac{1}{n} L_X^T H L_X + \gamma I \right) u
\]
where \( \gamma \) is the disentanglement regularization parameter defined in \( [9] \) and the supremum value of (12) is \( \sum_{j=1}^r \lambda_j \).

**Proof.** Consider the Cholesky factorization \( K_e = L_e L_e^T \) where \( L_e \) is a full row-rank matrix. Using representer theorem, disentanglement condition in (10), can be expressed as
\[
\text{Cov}(f_i(X), f_j(X)) = \gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}
\]
\[
= \frac{1}{n} \sum_{k=1}^n f_i(X_k)f_j(X_k) - \frac{1}{n^2} \sum_{k=1}^n f_i(X_k) \sum_{m=1}^n f_j(X_m) + \gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}
\]
\[
= \frac{1}{n} \sum_{k=1}^n \sum_{i=1}^n K_X(X_k, X_i) \theta_{it} \sum_{m=1}^n K_X(X_k, X_m) \theta_{jm} - \frac{1}{n^2} \theta_i^r K_X 1_n^T K_X \theta_j + \gamma \langle f_i, f_j \rangle_{\mathcal{H}_X}
\]
\[
= \frac{1}{n} (K_X \theta_i^r)^T (K_X \theta_j) - \frac{1}{n^2} \theta_i^r K_X 1_n^T K_X \theta_j + \gamma \left( \sum_{k=1}^n \theta_{ik}k_X(\cdot, X_k), \sum_{t=1}^n \theta_{it}k_X(\cdot, X_t) \right)_{\mathcal{H}_X}
\]
\[
= \frac{1}{n} \theta_i^r L_X^T (L_X^T H L_X + n \gamma I) L_X^T \theta_j
\]
\[
= \delta_{i,j}.
\]

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 \( V = L_X^T \Theta^T \) and consider the optimization problem in (13):
\[
\sup_{f \in \mathcal{A}_r} \left\{ (1 - \tau) \text{dep}_F^\text{emp}(f(X), Y) - \tau \text{dep}_F^\text{emp}(f(X), S) \right\}
\]
\[
= \sup_{f \in \mathcal{A}_r, \ n^2} \left\{ (1 - \tau) \| \Theta K_X H L_Y \|_F^2 - \tau \| \Theta K_X H L_S \|_F^2 \right\}
\]
\[
= \sup_{f \in \mathcal{A}_r, \ n^2} \frac{1}{n^2} \left\{ (1 - \tau) \text{Tr}(\Theta K_X H K_Y H K_X \Theta^T) - \tau \text{Tr}(\Theta K_X H K_S H K_X \Theta^T) \right\}
\]
\[
= \max_{V^T CV = I_r, \ n^2} \frac{1}{n^2} \text{Tr}(\Theta L_X B L_X^T \Theta^T)
\]
\[
= \max_{V^T CV = I_r, \ n^2} \frac{1}{n^2} \text{Tr}(V^T B V)
\]

(27)
where the second step is due to (9) and

\[ B := L_X^T \left( (1 - \tau)HKY - \tau HK_S \right) L_X \]

\[ = L_X^T \left( (1 - \tau)\tilde{K}_S - \tau \tilde{K}_S \right) L_X. \]

It is shown in [53] that an optimizer of (27) is any matrix \( U \) whose columns are eigenvectors corresponding to \( r \) largest eigenvalues of generalized problem

\[ Bu = \lambda Cu \]  

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 \( \Theta^{opt} \)). Note that \( \Theta^{opt} \) 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 \( \Theta^{opt} = U^T (L_X)^{\dagger} \).

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

\[ \arg \sup_r \left\{ \sup_{f \in \mathcal{A}_r} \{ J_{emp}(f(X)) := (1 - \tau) \text{dep}_{emp}(f(X), Y) - \tau \text{dep}_{emp}(f(X), S) \} \right\}, \]

which is the number of positive eigenvalues of the generalized eigenvalue problem in (13).

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

\[ \sup_{f \in \mathcal{A}_r} \left\{ (1 - \tau) \text{dep}_{emp}(f(X), Y) - \tau \text{dep}_{emp}(f(X), S) \right\} = \sum_{j=1}^{r} \lambda_j, \]

where \( \{\lambda_1, \ldots, \lambda_n\} \) are eigenvalues of the generalized problem in (13) in decreasing order. It follows immediately that

\[ \arg \sup_r \left\{ \sum_{j=1}^{r} \lambda_j \right\} = \text{number of positive elements of } \{\lambda_1, \ldots, \lambda_n\}. \]

**F Proof of Theorem 5**

**Theorem 5.** Assume that \( k_S(\cdot, \cdot) \) and \( k_Y(\cdot, \cdot) \) are bounded by one and \( f_k^2(x_i) \) is bounded by \( M \) for any \( k = 1, \ldots, r \) and \( i = 1, \ldots, n \) for which \( f = (f_1, \ldots, f_r) \in \mathcal{A}_r \). For any \( n > 1 \) and \( 0 < \delta < 1 \), with probability at least \( 1 - \delta \), we have

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

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

**Proof.** Recall that in the proof of Lemma 3, we have shown that with probability at least \( 1 - \delta \), the following holds,

\[ |\text{dep}(Z, S) - \text{dep}_{emp}(Z, S)| \leq \sqrt{\frac{r^2 M^2 \log(6/\delta)}{a^2 n}} + O \left( \frac{1}{n} \right). \]

\(^6\) Optimal \( V \) is not unique.
Using the same reasoning, with probability at least $1 - \delta$, we have
\[
\left| \text{dep}(Z, Y) - \text{dep}^{\text{emp}}(Z, Y) \right| \leq \sqrt{\frac{r^2M^2 \log(6/\sigma)}{\alpha^2n}} + O \left( \frac{1}{n} \right).
\]

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

We complete the proof by noting that
\[
\sup_{f \in A_r} \left| J(f(X)) - J^{\text{emp}}(f(X)) \right| \leq \sup_{f \in A_r} \left| J(f(X)) - J^{\text{emp}}(f(X)) \right|.
\]

\[\square\]

**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 if largest eigenvalues of the generalized problem in equation (11). Then, there exist a linear regression on top of the representation $Z = f^*(X)$ that is as effective as Bayes prediction $E_Y[Y|X]$, i.e.
\[
\min_{W, b} \mathbb{E}_{X,Y} \left[ \|WZ + b - Y\|^2 \right] = \mathbb{E}_{X,Y} \left[ \|E_Y[Y|X] - Y\|^2 \right].
\]

We only proof this Theorem for empirical version due to the convergence of the empirical version to the population counterpart. The optimal Bayes predictor can be the the composition of the kernelized encoder $Z = f(X)$ and an affine regressor on top of it. More specifically, $\bar{Y} = Wf(X) + b$ can approach to the optimal Bayes predictor if we optimize $f, r$ (the dimensionality of $f$), $W$, and $b$ all together. Let $Z := [z_1, \ldots, z_n] \in \mathbb{R}^{r \times n}$ and $Y := [y_1, \ldots, y_n] \in \mathbb{R}^{d_Y \times n}$. Further, let $\tilde{Z}$ and $\tilde{y}$ be the centered (i.e. mean subtracted) version of $Z$ and $Y$, 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
\[
\min_{W} \frac{1}{n} \|\tilde{W}\tilde{Z} - \tilde{Y}\|^2_F = \frac{1}{n} \min_{W} \|\tilde{Z}^T W^T - \tilde{Y}^T\|^2_F,
\]
\[
= \min_{W} \|\tilde{Z}^T W^T - P_Z \tilde{Y}^T\|^2_F + \frac{1}{n} \|P_Z \tilde{Y}^T\|^2_F
\]
\[
= \frac{1}{n} \|P_Z \tilde{Y}^T\|^2_F = \frac{1}{n} \|\tilde{Y}\|^2_F - \frac{1}{n} \|P_Z \tilde{Y}^T\|^2_F,
\]
where $P_Z$ denotes the orthogonal projector onto the columns of $\tilde{Z}^T$ and a possible minimizer is $W_{\text{opt}} = (\tilde{Z}^T)\tilde{Y}^T$ 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 $P_Z = \frac{1}{n} \tilde{Z} \tilde{Z}^T$. Now, consider optimizing $f(X) = \Theta[k_X(x_1, X), \ldots, k_X(x_n, X)]^T$. We have, $\tilde{Z} = \Theta K_X H$ where $H$ is the centering
matrix. Let $\mathbf{V} = \mathbf{L}_X^T \Theta^T$ and $\mathbf{C} = \frac{1}{n} \mathbf{L}_X^T \mathbf{H} \mathbf{L}_X$

\[
\Theta \mathbf{K}_X \mathbf{H} \mathbf{K}_X \mathbf{H}^T = \frac{1}{n} \mathbf{P}_\tilde{\mathbf{Y}}^T \mathbf{P}_\tilde{\mathbf{Y}}^T
\]

\[
\Theta \mathbf{K}_X \mathbf{H} \mathbf{K}_X \mathbf{H}^T = \frac{1}{n} \mathbf{P}_\tilde{\mathbf{Y}}^T \mathbf{P}_\tilde{\mathbf{Y}}^T
\]

\[
\Theta \mathbf{K}_X \mathbf{H} \mathbf{K}_X \mathbf{H}^T = \frac{1}{n} \mathbf{P}_\tilde{\mathbf{Y}}^T \mathbf{P}_\tilde{\mathbf{Y}}^T
\]

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

\[
B_0 \mathbf{u} = \lambda \mathbf{C} \mathbf{u}
\]

and $B_0 := \mathbf{L}_X^T \tilde{\mathbf{Y}}^T \tilde{\mathbf{Y}} \mathbf{L}_X$. This is resembles the eigenvalue in Section E equation (28) 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 $d_Y$. 

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