Latent Variable Models for Bayesian Causal Discovery

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Abstract

Learning predictors that do not rely on spurious correlations involves building causal representations. However, learning such a representation is very challenging. We, therefore, formulate the problem of learning a causal representation from high dimensional data and study causal recovery with synthetic data. This work introduces a latent variable decoder model, Decoder BCD, for Bayesian causal discovery and performs experiments in mildly supervised and unsupervised settings. We present a series of synthetic experiments to characterize important factors for causal discovery.

1. Introduction

Exploiting structure in the data to infer latent variables and capture causal mechanisms is crucial for causal representation learning (Schölkopf et al., 2021). Such a representation would allow for counterfactual reasoning in a manner similar to that of humans, thereby moving away from models that rely on exploiting spurious correlations for prediction.

Causal mechanisms are usually modelled as Bayesian Networks or Directed Acyclic Graphs (DAG) and given information about the causal variables, one can learn the DAG with structure learning algorithms. Recently, there has been a flurry of works advancing structure learning algorithms (Lorch et al., 2021; Annadani et al., 2021; Cundy et al., 2021; Deleu et al., 2022; He et al., 2019; Ng et al., 2021; Zheng et al., 2018; Pamfil et al., 2020; Shimizu et al., 2006) that learn the structure of a DAG given data samples (of causal variables). Most of these works cast the discrete optimization of learning a DAG into a continuous one that is optimized through gradient descent, thereby sidestepping computational intractability arising from the super-exponential nature of DAG search in the discrete case. However, all approaches learn a causal DAG on the premise that one has full access to the true causal variables which might not be realistic. A more realistic assumption would be that we have partial or no access to true causal variables and that one has to infer the structure *along with* the causal variables.

Here, we use a fully differentiable latent variable model, Decoder BCD, to study the problem of Bayesian structure learning in linear Gaussian additive noise models, from high dimensional data. We perform synthetic experiments to analyze why unsupervised causal discovery in latent variable models is difficult. Section 2 explains preliminaries for the setup and section 3 gives the problem setup. In section 4, we introduce Decoder BCD, a decoder model for Bayesian Causal Discovery in the latent space before discussing experiments and our findings in section 5. We discuss related work in section 6 before concluding in section 7.

2. Preliminaries

Structural Causal Models (SCM): We operate in the framework of SCM (Pearl, 2009) where node Z_i represents a random causal variable with an independent noise variable $\epsilon_i \sim \mathcal{N}(0, \sigma_i^2)$, and parents $Pa_G(Z_i)$ corresponding to a DAG G. We focus primarily on the family of linear Gaussian additive noise models. However, for a DAG to be identifiable from data, one either has to observe a non-Gaussian setting, or, in the case of a Gaussian one, have an equal noise variance assumption (all $\sigma_i = \sigma$) (Peters & Buhlmann, 2014). Since we are in the Gaussian setting, we assume the latter. Thus, we have d causal variables $Z = [Z_1, ...Z_d]$, and a joint distribution entailed by the DAG G such that,

$$P(Z_1, ...Z_d) = \prod_{i=1}^{d} P(Z_i | Pa_G(Z_i)) \tag{1}$$

and the exact values of the d random variables are given by $z_i = f(Pa_G(z_i)) + \epsilon_i$, where $f(.)$ is a linear function. In our case, f is the weighted sum of values taken on by random variables $Pa_G(Z_i)$, the weights given by the weighted adjacency matrix W, such that $z = W^T z + \epsilon$.

Bayesian Causal Discovery Nets (BCD Nets): We build Decoder BCD, our latent variable decoder model, upon BCD Nets (Cundy et al., 2021). Given samples of true causal variables, BCD Nets is a Bayesian structure learning method that obtains a posterior distribution over causal

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structures that best explains the data. Similar to other structure learning works (Lorch et al., 2021), BCD Nets introduces the problem of structure learning as a continuous constrained optimization problem. However, the DAG is parameterized such that one always ends up with a DAG and is therefore a hard constraint (in contrast to DiBS which has a soft DAG constraint). This is achieved by formulating the weighted adjacency matrix as $W = (PLP^T)^T$ where P is a permutation matrix and L is strictly lower triangular. When P is identity, this is equivalent to having a DAG of fixed ordering with each node j having its possible parents only in the node range $[j+1, d]$. P allows one to transition between node orderings by permuting the rows and columns of L. Apart from estimating W (via P and L), BCD Nets also infers Σ, the noise covariance, for the noise variables on each node in the DAG.

Thus, overall, BCD Nets formulates the Bayesian Structure Learning problem as inference of P, L, and Σ with a unique factorization of the posterior as $q_\phi(P, L, \Sigma) = q_\phi(P|L, \Sigma) \cdot q_\phi(L, \Sigma)$. The model is trained on an ELBO loss (eq. 2) with a horseshoe prior on L, Gumbel Sinkhorn prior (Jang et al., 2016) on P, and a Gaussian prior on Σ.

$$\mathbb{E}_{(L,\Sigma)\sim q_\phi}\Big[\mathbb{E}_{P\sim q_\phi(.|L,\Sigma)}\big[\log p(X|P,L,\Sigma) - \log \frac{q_\phi(P|L,\Sigma)}{p(P|L,\Sigma)}\big] - \log \frac{q_\phi(L,\Sigma)}{p(L,\Sigma)}\Big] \tag{2}$$

For finer details, we refer the reader to the original work (Cundy et al., 2021). Our work focuses more on *extending* BCD Nets to the high dimensional setting and studying unsupervised graph recovery in the latent space.

3. The Problem Setup

This work revolves around the Bayesian inference of causal variables Z and the causal structure G. Given n samples of high dimensional data $X \in \mathbb{R}^{n\times D}$, we wish to recover a distribution over graph structures G – the (weighted) adjacency matrix – and the causal variables $Z \in \mathbb{R}^{n\times d}$. Our setup revolves mostly around the recovery in linear isotropic Gaussian additive noise SCM, which is identifiable. Models like DiBS (Lorch et al., 2021), VCN (Annadani et al., 2021), and BCD Nets (Cundy et al., 2021) can recover the Ground Truth (GT) DAG given only observational and interventional data. Given observational data, recovery is possible up to a Markov Equivalence Class (MEC).

We first generate a random ER (Erdös & Rényi, 1959) DAG — with weighted adjacency matrix W_{GT} with sparsity pattern G_{GT}, the adjacency matrix — and consider this the ground truth and set the noise covariance to be $\Sigma_{GT} = \sigma^2_{GT} I$, since we have an isotropic Gaussian assumption. In our experiments, σ_{GT} is usually set to 0.1.

Data generation of the true causal variables: The data generation is done by an ancestral sampling process, compactly given by $z = W^T z + \epsilon$. One could also get interventional data from this setup: **(i)** Choose the node set N being intervened upon, **(ii)** for every node in N, zero out the particular column in W to get the mutated DAG $\tilde{W}$ and **(iii)** perform ancestral sampling using $z = \tilde{W}^T z + \epsilon$. This process is repeated multiple times to get n samples of z, and we will then organize these samples into a (n, d) matrix and term it z_{GT}, or simply, z [1].

Generating the true high dimensional data: We assume the observed low level data is a linear projection of the causal variables given by $X_{GT} = z_{GT} P'$, where $P' \in \mathbb{R}^{d\times D}$ is a projection matrix and we have $D >> d$ in the real world. For most of the upcoming experiments, we will study recovery in the (simpler) limiting case where d equal to D. This work studies recovery in latent space in a case where direct access to true causal variables is not given, in contrast to existing structure learning works.

4. Decoder BCD

BCD Nets performs Bayesian inference over P, L, Σ given samples of true causal variables to best explain the data by training an ELBO loss (see eq. 2). Decoder BCD tries to infer the decoder parameters in addition to inferring P, L, Σ. It is trained over X_{GT} instead of over z_{GT} as in BCD Nets. Thus, we relax the assumption that we have access to samples of true causal variables. We can only access the high dimensional data that has to be explained by (Z, G) and we have to fit a structure, $\hat{G}$, and estimate edge weights, $\hat{W}$, to fit our best guess of the causal variables, $\hat{z}$. Algorithm 1 summarizes the inference mechanism of Decoder BCD.

Algorithm 1 Decoder BCD for causal discovery from high dimensional data

1. Initialize random distributions for P, L, Σ
2. For **train_steps**:

(i) Sample $\hat{P}, \hat{L}, \hat{\Sigma} \sim q_\phi(P, L, \Sigma)$
(ii) $\hat{W} = (\hat{P}\hat{L}\hat{P^T})^T$
(iii) Generate $\hat{z} = \hat{W}^T \hat{z} + \epsilon$; $\epsilon \sim \mathcal{N}(0, \hat{\sigma})$ and $\hat{\Sigma} = \hat{\sigma}^2 I$
(iv) Decode $\hat{z}$ to obtain $\hat{X}$
(v) Update parameters of the distribution $P(P, L, \Sigma)$ with loss as $MSE(X, \hat{X})$
(vi) For supervised experiments, add an additional KL loss between true and posterior observational joint: $KL(q(z_1, ...z_d)||p(z_1, ...z_d))$

[1] These variables will also be referred to, at times, as samples of true causal variables

5. Experiments and Findings

For all our experiments, for simplicity, we will stick to just learning the decoder and inferring the edge matrix L since this makes the optimization simpler for our studies. Such an assumption of fixing the permutation P to the GT, and thereby, the node orderings, is not unreasonable (He et al., 2019). Here, the focus is solely on inferring the edges L in latent space whilst learning a decoder. In all experiments, we train the model for 5000 steps across 20 random seeds, with a learning rate of 0.002 on ER-2 DAGs.

Metrics: In our experiments, we refer to the expected Structural Hamming Distance across 64 samples of the inferred DAG as SHD, **L_MSE** is the MSE between predicted $\hat{L}$ and L_{GT}, AUROC (a value of 0.5 denotes a random baseline with null edges), and **obs_KL_term_Z** refers to the KL divergence between the posterior observational joint and the GT observational joint distributions.

5.1. Learning edge matrix L with supervision

For the supervised experiments, we add an additional KL loss on the inferred posterior observational joint $q(z_1, ...z_d)$ and the prior observational GT joint distribution, $p(z_1, ...z_d) \sim \mathcal{N}(\mu_z, \Sigma_z)$, where Σ_z is calculated with W_{GT} instead of with $\hat{W}$. The estimation of the prior and posterior observational joint distribution is detailed in A.1.

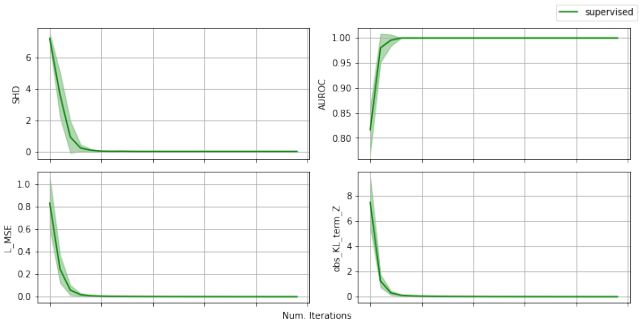

Figure 1. Supervised learning of L with the MSE+KL loss on 600 observational data points with $d = 6, D = 10$

Finding 1: From figure 1, we can see the expected SHD approaching 0 as the KL term (denoted **obs_KL_term_Z**) and **L_MSE** approach 0. KL over the observational joint distribution results in complete graph recovery in the supervised case. This is expected since we provide a mild signal for the model to uncover the true causal variables. Instead of providing prior over the samples of true causal variables, we use the observational joint distribution as a signal.

5.2. Unsupervised learning of a single edge weight

For this setting, instead of inferring the whole lower triangular edge matrix L, we infer only the last edge at position $(d, d-1)$. The other elements of the matrix are fixed to the GT and we observe graph recovery in this case. This subsection is split into two parts to study recovery with (i) observational data and (ii) a mix of observational and interventional data, to analyze the effects of interventional data. We use 1800 observational data points for case (i) and 1800

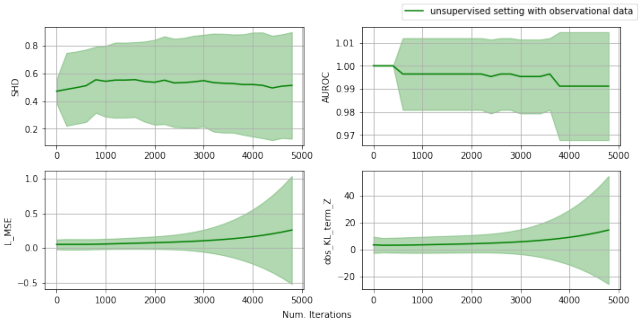

Figure 2. Unsupervised learning of a single edge weight with 1800 observational data points

data points (50-50 split of observational and interventional data) for case (ii). For training, we project this d =6 node DAG to D =10 dimensions. The interventional data generation process for single node and multi node interventions is detailed in A.2. **Finding 2**: Figures 2 and 3 reveal that

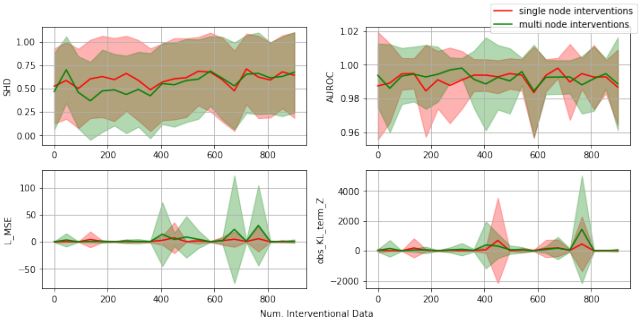

Figure 3. Unsupervised learning of a single edge weight with 900 observational and 900 interventional data points

using observational and/or interventional data with single node or multi node interventions is not sufficient to learn to orient a single edge in the unsupervised case.

5.3. Unsupervised learning of edge weight L

In this experiment and in the next, we explore the problem of learning the entire lower triangular edge matrix L in an

unsupervised setting. First, we consider the learning problem with various amounts of observational data to analyze its effect on edge recovery in the latent space, which is shown in figure 4.

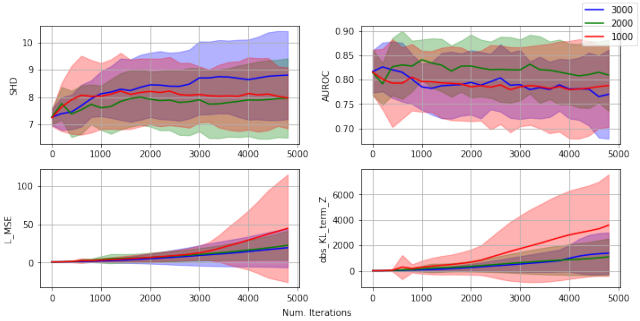

Figure 4. Unsupervised learning of the edge weight matrix with various amounts of observational data

Finding 3: Figure 4 shows that all metrics diverge with training, but graph recovery seems to diverge lesser with more observational data, for example, blue (3k) $<$ green (2k) $<$ red (1k) along **L_MSE** and **obs_KL_term_Z**. We find these to be better metrics for evaluation since they are continuous measures, rather than SHD, a discrete metric. Moreover, SHD is independent of the edge weight and only depends on the direction of the edge.

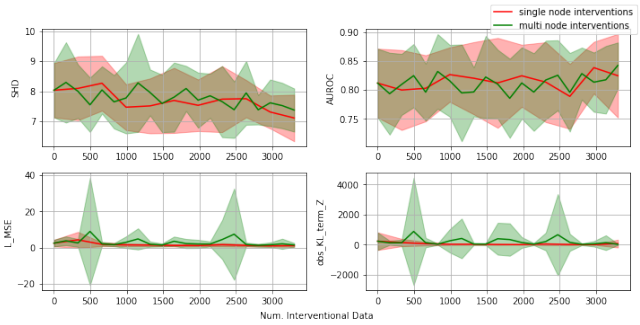

Figure 5. Unsupervised learning of the edge weight matrix with single node and multi node interventions

We now consider learning L using interventional targets as labels to learn the structure in the latent space with a mix of 300 observational data points and 3300 interventional data points. For this experiment, we retrain Decoder BCD multiple times from scratch — each time with the same 300 observational data points but with more interventional data than the previous run. This helps us understand the usefulness of interventional data for graph recovery. This result is illustrated in figure 5.

Finding 4: Figure 5 shows that both single node and multi node interventions help in recovering the edge weights, measured across all the 4 metrics. However, one might prefer single node interventions (red) due to lesser variance across the **L_MSE** and **obs_KL_term_Z** metrics. This might be due to single node interventions having more data points *per* intervention.

6. Related Works

To address the challenges of causal discovery, a variety of methods have been proposed. Some of these methods are based on structure learning using observational data and some take in to account interventional data (Lorch et al., 2021; Scherrer et al., 2021; Ke et al., 2019; Brouillard et al., 2020).

There has been an increasing focus on Bayesian structure learning (Annadani et al., 2021; Lorch et al., 2021; Cundy et al., 2021; Deleu et al., 2022; Yu et al., 2019) to quantify epistemic uncertainty that is crucial for reinforcement learning and active learning settings. There also exist many maximum likelihood based methods, one such example is (He et al., 2019). It is one of the few works that learn a structure in the latent space but they do not operate in a causality or SCM framework.

Markov Chain Monte Carlo (MCMC) is a popular technique for sampling from complex high dimensional probability distributions, such as the posterior distribution of DAGs. (Madigan et al., 1995) uses Metropolis-Hastings (Metropolis et al., 1953) to predict the posterior distribution through Markov space to perform single edge addition or deletion. (Eaton & Murphy, 2007) propose a hybrid MCMC algorithm that uses an exact score based algorithm. (Kuipers et al., 2022) and (Viinikka et al., 2020) use more efficient MCMC samplers. (Deleu et al., 2022) uses a novel class of probabilistic models, GFlowNets (Bengio et al., 2021), to approximate the posterior in place of MCMC algorithms. Section A.3 discusses related work in more detail.

7. Conclusion

In this work, we introduced our latent variable model, Decoder BCD, and studied the causal representation learning problem. We explored the cases where edge recovery fails – learning to orient a single edge or learning with only observational data. To address this, we propose using interventional targets as labels to better learn the entire edge matrix, and show that this is a promising direction for the unsupervised setting. However, our hypothesis of the observed data being a linear projection of the latent causal variables to a higher dimension is a limitation (refer A.5). Future work should explore non-linear projections of the causal variables. Finally, we discuss some key challenges for future study in Appendix A.4.

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A. Appendix

A.1. KL Loss for the mildly supervised experiments

Given $\hat{W} = (P\hat{L}P^T)^T$, from inferred $\hat{L}$, one can obtain the mean and covariance of the observational joint distribution $q(z_1, ...z_d)$ as follows:

$$z = \hat{W}^T z + \epsilon; \quad \epsilon \sim \mathcal{N}(0, \sigma) \tag{3}$$

$$z = (I - \hat{W})^{-T}\epsilon \tag{4}$$

$$q(z_1, ...z_d) \sim \mathcal{N}(\hat{\mu_z}, \hat{\Sigma_z}) \tag{5}$$

$$\hat{\mu_z} = 0 \; and \; \hat{\Sigma_z} = (I - \hat{W})^{-T}\Sigma(I - \hat{W})^{-1} \tag{6}$$

To estimate the prior GT observational joint distribution, one would use W in place of $\hat{W}$ in equation 6.

A.2. Generating interventional data for experiments that use single node and multi node interventions

Suppose we have to generate i interventional data points. We split the data generation process into $s = 20$ sets, each set generating i/s interventional data points. *For single node interventions*, we randomly choose a node and sample i/s data points. The process is repeated s times randomly to generate the i data points. *For multi node interventions*, we randomly choose a number between [2, d] to decide on the number of nodes to intervene on (call this x). We then choose x nodes without replacement and perform the interventions on these nodes and sample i/s data points. The process is repeated s times randomly to generate the i data points.

A.3. More Related Work

Since discrete optimization is hard and often involves enumeration of possible structures, the super-exponential nature of structure learning has resulted in the community resorting to relaxing the discrete optimization problem into a continuous one (Lorch et al., 2021; Cundy et al., 2021; Annadani et al., 2021; Scherrer et al., 2021; Ke et al., 2019; Zheng et al., 2018) and learning the parameters using gradient descent. (Loh & Bühlmann, 2013) propose a scalable, scoring-based DAG learning approach to recover high dimensional, sparse causal graphs in a non-Gaussian setting where only some but not all exogenous noise variables are expected to be non-Gaussian. (Ghoshal & Honorio, 2017) learns a linear structural equation model in polynomial time. (Ke et al., 2019) learns the causal structure from unknown interventions but operates on the Bernoulli distribution while (Scherrer et al., 2021) is in an active learning framework and the system determines the intervention that will be most useful in gaining knowledge about the graph structure. (Yang et al., 2020) proposes a variational autoencoder parameterised by exogenous variables to learn causal semantics of the data. Another family of works introduce assumptions to functional and parametric form of the data-generation structure. They exploit symmetries to learn the causal structure (Peters et al., 2017; Mooij et al., 2016).

Approaches to the problem are mostly employ score-based or constraint-based optimization. Most modern methods use some sort of a scoring function to rank estimated structure and use it to rank structures and optimizing for the score is expected to return the ground truth DAG. Popular scoring functions include Bayesian Information Criterion (BIC) and BGe score (Geiger & Heckerman, 1994). These methods typically use a regularization over the structure to induce sparsity and/or acyclicity. Some methods impose hard constraints as well that ensure the search is done only over the space of DAGs. (Shah & Peters, 2020) is a constraint based approach that tests for conditional independence.

A.4. Key challenges for future study

Unsupervised learning of causal variables: Our aim is to uncover a causal representation consisting of variables z and a structure G thereof. Given the right causal variables z, methods exist to uncover a graph structure G that explains the observed data. However, a bottleneck in learning this joint representation is that we need a signal to guide the search space as we are looking for good candidates for causal variables z. We currently use distributional information of z_{GT} to guide the

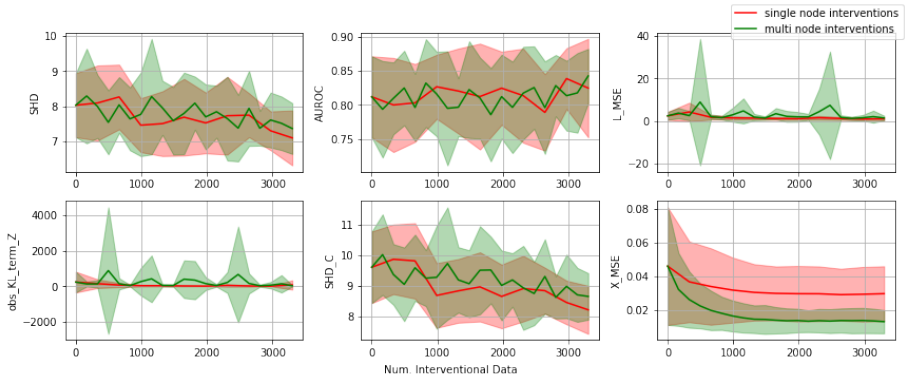

Figure 6. Unsupervised learning of the edge weight matrix with single node and multi node interventions

learning of z, but one should look out for methods with subtler or no supervision. Thus, an important challenge is "can we learn causal variables with little to no supervision?". In an attempt to solve this, we tried using interventional data and the interventional targets as labels to understand whether it would help provide a signal to learn the right causal variables. From our experiments, this seems to help the structure learning problem.

One of the most important scientific questions of causal representation learning is regarding the **relationship between high dimensional, observed variables and the low dimensional, causal variables**: In this work, we perform synthetic data generation of z and project it to higher dimensions by using a random projection matrix P'. We begin on the premise that real-world, high dimensional data can be explained by a few causal variables and the inferring these variables and their structure is the problem of causal inference that the brain solves for performing intelligent tasks. Thus, there must exist an operation that maps the low dimensional causal variables to the high dimensional, observed variables (eg. images, videos). For our problem setting, we assume this is true and try to generate high dimensional samples that are "causally consistent" by performing a linear projection $X = zP'$. However, we do not know how this process of projection to higher dimensions might happen in reality.

What's the right loss function for unsupervised causal discovery? In all experiments, we found that the MSE over high dimensional data, X, goes down but this does not necessarily mean that graph recovery in the latent space gets better (measured along **L_MSE** or **obs_KL_term_Z**). Therefore, we need to look for alternative losses with a property such that reduction in loss over X guarantees a better recovery in the latent space (i.e., better graph structure recovery or better estimates of edge weight matrix L). Ideally, such a loss should result in a reduction in **obs_KL_term_Z** which measures the KL divergence between the inferred posterior observational joint distribution and the GT observational joint distribution. We propose that this a better metric to measure since in the supervised experiments, getting a low enough value of this metric results in the SHD dropping steeply to 0.

A.5. Limitations

A limitation of this work is that we do not know if it is practical to assume a linear projection – it is just a formulation that we explore. Additionally, if it *is* a linear operation, are there any properties that the projection matrix P' must hold to maintain this "causal consistency" in higher dimensions? If P' needs to hold some properties for causal inference to be performed from high dimensions, *what* exactly are these properties? It is easy to see that a random projection matrix (which transforms a d-dimensional vector to D-dimensional vector) can be random enough to completely destroy the encoded information due to the causal generation process that occurred in the lower dimensions, and thus the high dimensional data could no longer be "causally consistent" for us to perform inference. And finally, one needs to focus on the question of whether the projection operation could be nonlinear.