Entropic Latent Variable Discovery

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Abstract

We consider the problem of discovering the simplest latent variable that can make two observed discrete variables conditionally independent. This problem has appeared in the literature as probabilistic latent semantic analysis (pLSA), and has connections to non-negative matrix factorization. When the simplicity of the variable is measured through its cardinality (Renyi entropy with $\alpha = 0$), we show that a solution to this latent variable discovery problem can be used to distinguish direct causal relations from spurious correlations among almost all joint distributions on simple causal graphs with two observed variables. Conjecturing a similar identifiability result holds with Shannon entropy, we study a loss function that trades-off between entropy of the latent variable and the conditional mutual information of the observed variables. We then propose a latent variable discovery algorithm — \textit{LatentSearch} — and show that its stationary points are the stationary points of our loss function. We experimentally show that LatentSearch can indeed be used to distinguish direct causal relations from spurious correlations.

1 Introduction

Consider the following problem: we are given two discrete random variables $X, Y$ over $m$ and $n$ states respectively. Suppose we want to construct a third random variable $Z$, such that $X$ and $Y$ are independent conditioned on $Z$. Without any constraints this can be trivially achieved: Simply picking $Z = X$ or $Z = Y$ ensures that $X \perp \perp Y | Z$. However, this requires that the random variable $Z$ is as complex as $X$ or $Y$. We therefore ask the following question: \textit{is there a simple $Z$ that makes $X, Y$ conditionally independent?} Suppose we measure the complexity of $Z$ by its cardinality (equivalently, its Renyi entropy for $\alpha = 0$). Then, a non-trivial answer to this question would require us to find a random variable $Z$ with $k$ states, where $k < \min\{m, n\}$ that renders $X, Y$ conditionally independent. This problem of recovering a small cardinality latent variable $Z$ is closely related to Probabilistic Latent Semantic Analysis (pLSA), non-negative matrix factorization (NMF) and Latent Dirichlet Allocation (LDA). In this paper we show that a solution to this problem can also be used for causal inference in the presence of latent variables: Suppose, given two dependent random variables $X, Y$, that our objective is to decide if there is a direct causal relation between the two, or if the observed correlation is spurious, i.e., due to an indirect path via a latent variable.

Our main theoretical result is that it is always possible to distinguish the latent causal graph from the triangle causal graph (see Figure [I]) where $Z$ is latent, if the latent variable has \textit{cardinality (aka Renyi entropy for $\alpha = 0$)} less than $\min\{m, n\}$, except for a measure zero set of joint distributions.
We also study this problem using an alternate simplicity metric of Shannon entropy instead of cardinality. In this case, our problem becomes: Given two discrete variables $X, Y$ with $m, n$ states, respectively, what is the minimum entropy variable $Z$ with $k$ states that assures $X \perp \perp Y \mid Z$? We conjecture that an identifiability result also holds in this case even when $k \geq n$, thus permitting us to study a larger class of latent $Z$. More precisely, we expect most distributions generated from the triangle graph with small entropy $Z$ to require a large entropy $Z$ to satisfy conditional independence $X \perp \perp Y \mid Z$.

With these observations, our main algorithmic contribution is as follows: To solve the problem of recovering the minimum entropy $Z$ that renders the observed variables $X, Y$ conditionally independent, we propose an algorithm to minimize the loss $I(X; Y \mid Z) + \beta H(Z)$. The parameter $\beta$ allows us to discover a tradeoff between the simplicity of variable $Z$ and how much of the dependence between $X, Y$ it can explain away. We show that our algorithm always outputs a stationary point of the loss function. Moreover, for $\beta = 1$, we are able to show convergence of the algorithm, and that it converges to either a local minimum or a saddle point. We also empirically demonstrate that it converges much faster than gradient descent and recovers better solutions after convergence.

Our contributions are as follows:

- Given a joint dist. between two discrete variables $X, Y$, we propose LatentSearch – a latent variable discovery algorithm that constructs a third variable $Z$ to minimize $I(X; Y \mid Z) + \beta H(Z)$.

- We show that the stationary points of our algorithm are also stationary points of the loss $I(X; Y \mid Z) + \beta H(Z)$. For $\beta = 1$, we prove convergence and show that the algorithm converges to either a local minimum or a saddle point.

- Using our algorithm, we empirically demonstrate a fundamental tradeoff between the discovered latent variable’s complexity, measured by its entropy, and how much of the dependence between the observed variables it can explain away.

- We show that if we are given an algorithm that recovers the variable $Z$ with minimum number of states, this algorithm can be used to distinguish the two causal graphs $X \leftarrow Z \rightarrow Y$ from $X \leftarrow Z \rightarrow Y, X \rightarrow Y$, where $Z$ is latent. We conjecture that the identifiability result holds if we use Shannon entropy of the variable, instead of its cardinality.

- We use our latent variable discovery algorithm to test the validity of our conjecture on simulated data and show that the true causal graph is identifiable even when $k \geq n$ with probability close to 1.

- Our latent variable discovery algorithm can be used to answer the question: *Is the causal relation between two given variables direct, or is there a simple variable conditioned on which, they become independent.* Based on this, we use our algorithm on Ad*ult dataset from UCI repository [5] to recover the skeleton of the causal graph. We show that, for a carefully chosen entropy threshold for the unobserved variables, our algorithm recovers almost the exact skeleton as the BIC score based structure learning algorithm.

2 Background and Notation

Let $D = (\mathcal{V}, E)$ be a directed acyclic graph on the set of vertices $\mathcal{V} = \{V_1, V_2, \ldots, V_n\}$ with directed edge set $E$. Each directed edge is a tuple $(V_i, V_j)$, where $V_i, V_j \in \mathcal{V}$. Let $\mathcal{P}$ be a joint distribution over a set of variables labeled by $\mathcal{V}$. $D$ is called a valid Bayesian network for the distribution $\mathcal{P}$ is
the distribution factorizes with respect to the graph as $P(V_1, V_2, \ldots V_n) = \prod_i P(V_i|pa_i)$, where $pa_i$ are the set of parents of vertex $V_i$ in graph $D$. If $D$ is a valid Bayesian network for $P$, if the three vertices $X, Y, Z$ satisfy a purely graphical criterion called the d-separation, $X \perp \perp Y | Z$ with respect to $P$. A distribution $P$ is called faithful to graph $D$ if the converse is also true: Any three variables such that $X \perp \perp Y | Z$ satisfy the d-separation criterion on graph $D$.

Note that the edges in a Bayesian network do not carry a physical meaning: They simply indicate how a joint distribution can be factorized. Causal Bayesian networks (or causal graphs\textsuperscript{1}) extend the notion of Bayesian networks to different experimental, the so called interventional settings. An intervention is an experiment that changes the workings of the underlying system and sets the value of a variable, shown as $do(X = x)$. Causal Bayesian networks allow us to calculate the joint distributions under these experimental conditions, called the interventional distributions\textsuperscript{2}.

In this paper, we will work with the simple causal graphs given in Figure 1. From the d-separation principle, we see that the latent graph satisfies $X \perp \perp Y | Z$, whereas under the faithfulness condition, $X \not\perp \perp Y | Z$ in the triangle graph. Checking the existence of such a latent variable can help us recover the true causal graph as we discover in the next sections.

In this paper, we work with discrete ordinal or categorical variables. Suppose the cardinalities of the observed variables $X, Y$ are $m, n$, respectively. The joint distribution can be then be represented with an $m \times n$ non-negative matrix whose entries sum to 1. We assume that we have knowledge of this joint distribution (of the pair of observed variables).

We use $[n]$ to represent the set $\{1, 2, \ldots, n\}$ for any positive integer $n$. Capital letters are used to represent random variables whereas lowercase letters are used to represent realizations unless otherwise stated\textsuperscript{3}. Letters $X, Y$ are reserved to represent the observed variables, whereas letter $Z$ is used to represent the latent variable. To represent the probability mass function over three variables $X, Y, Z$, we use $p(x, y, z) := P(X = x, Y = y, Z = z)$ and similarly for any conditional $p(z|x, y) := P(Z = z|X = x, Y = y)$. Lowercase boldface letters are used for vectors and uppercase boldface letters are used for matrices. We also use $p(Z|x, y)$ to represent the conditional probability mass function $P(Z|X = x, Y = y)$ (Similarly for $p(Z|x), p(Z|y)$). $\text{card}(X)$ stands for the cardinality of the size of $X$’s support. Entropy of a random variable $X$, shown via $H(X)$, refers to its Shannon entropy, measured as $H(X) = -\sum_x p(x) \log(p(x))$.

\begin{figure}[h]
\centering
\begin{subfigure}{0.4	extwidth}
\centering
\begin{tikzpicture}
\node at (0,0) (X) {$X$};
\node at (1,0) (Y) {$Y$};
\node at (0.5,1) (Z) {$Z$};
\draw (X) -- (Z);
\draw (Y) -- (Z);
\end{tikzpicture}
\caption{Latent graph}
\end{subfigure}
\begin{subfigure}{0.4	extwidth}
\centering
\begin{tikzpicture}
\node at (0,0) (X) {$X$};
\node at (1,0) (Y) {$Y$};
\node at (0.5,1) (Z) {$Z$};
\draw (X) -- (Y);
\draw (X) -- (Z);
\draw (Y) -- (Z);
\end{tikzpicture}
\caption{Triangle graph}
\end{subfigure}
\caption{Causal graphs we want to distinguish. $Z$ is latent (unobserved).}
\end{figure}

\textsuperscript{1}In this work, we do not use structural causal models, hence causal graph refers to causal Bayesian networks.

\textsuperscript{2}Due to space constraints, we cannot formally introduce Pearl’s framework. Please see\textsuperscript{[18, 15]}.

\textsuperscript{3}In the supplementary material, $x_i$ is used to represent the probability that variable $X$ takes the value $i$. 
3 Related Work

Tools for Latent Variable Discovery: Latent variables have been used to model and explain dependence between observed variables in different communities under different names. One of the first models is the probabilistic latent semantic analysis (pLSA) framework developed by [7]. Given two variables $X, Y$ pLSA constructs a variable $Z$ that makes the two variables conditionally independent via two equivalent formulations. These two formulations correspond to fitting either the Bayesian network $X \rightarrow Z \rightarrow Y$ or $X \leftarrow Z \rightarrow Y$. pLSA is solved by running EM algorithm. However it does not have an incentive to discover low-entropy latents. In Section 6 we will see that running EM on top of our algorithm cannot help discover better solutions for our problem.

Latent Dirichlet allocation (LDA) is another framework for latent variable discovery, which has been widely used especially in topic modeling [2,11]. It is developed for creating a generative model of a given set of documents. Given $m$ documents each with a collection of words out of a dictionary with $n$ words, LDA recovers a factorization of the word count matrix $M = UV$, where the columns of $V$ are the mixtures of topics for each document. When the prior of these mixtures is chosen from a Dirichlet distribution with parameter less than 1, it encourages low entropy columns for $V$. However notice that when we map LDA to our setting, this does not correspond to the entropy of the latent variable: The distribution of the latent variable can be obtained from the LDA decomposition as the row sums of the matrix $V$, which can have large entropy even if columns of $V$ are 1 sparse.

Non-negative matrix factorization is another approach that can be seen as explaining the observed dependence between two variables with a simple latent factor. Compared to PCA, NMF explains the data with non-negative factors. Given a matrix $M$, NMF approximates it as $M \approx UDV$, where $U, D, V$ are $m$-by-$k,k$-by-$k,k$-by-$n$ non-negative matrices, respectively and $D$ is a diagonal matrix. Factorizing the joint distribution matrix between two observed variables via NMF with generalized KL divergence loss recovers solutions to the pLSA problem [6]. NMF, in general, is not unique.

Perhaps the most relevant to ours are the two papers in the Bayesian setting [3,17]. They use low-entropy priors on the latent variable’s distribution while performing inference. However their approach is different and their methods cannot be used to discover the tradeoff between unexplained away dependence and complexity of the latent variable as we do. In [17], the authors use low-entropy prior as a proxy for discovering latent factors with sparse support.

Our approach is also related to the information bottleneck principle. There, the authors propose an iterative algorithm to construct the conditional probability distribution of $Z|X$ for the Markov chain $Y \rightarrow X \rightarrow Z$, where $X,Y$ are observed. Their objective is to make sure $Z$ is as informative as possible about $X$, while being the least informative about $Y$. Accordingly, they propose an algorithm that after convergence outputs a stationary point of the loss function $L = I(X; Z) − \lambda I(Y; Z)$.

Learning Causal Graphs with Latents: Learning causal graphs with and without latent variables has been extensively studied in the literature. In graphs with many observed variables, although many of the causal edges can be recovered from the observational data (for example through algorithms that employ CI (conditional independence) tests such as IC [15], PC [18]), some of the causal edges are not identifiable unless one performs experiments and collects additional data. The existence of latent variables make the problem even harder. Although extensions of these algorithms can be employed (IC*, FCI and derivatives), in general, fewer number of edges can be learned due to the confounding that cannot be controlled for: Latent variables make the CI tests less informative, by inducing spurious correlations between the observed variables. Especially, even in the simple case when we want to decide between the latent and triangle graphs in Figure 1 these CI based algorithms cannot be used.

Our approach is, in essence, similar to [11]. There, the authors assume that the unobserved background variables have small entropy and suggest an algorithm to distinguish between the causal
graphs $X \to Y$ and $X \leftarrow Y$. Our setup is also similar to the one in [10], where they identify a condition on the conditional distribution $p(Y|X)$ that, if true, implies that there does not exist any simple latent variable $Z$ that can make $X, Y$ conditionally independent. This assumption, in the discrete variable setup, roughly implies that the matrix $p(X, Y)$ is sparse in a structured way. In the continuous variable setting, [10] propose using kernel methods combined with a rank argument to detect latent confounders between two variables. [20] analyzes the discoverability of causal structures with latents using the entropic vector of the variables. Finally, related work also includes [9] and [12], where the authors extend the additive noise model based approach in [8] to the case with a latent confounder.

### 4 LatentSearch: An Algorithm for Latent Variable Discovery

We formulate the problem of discovering the latent variable with small entropy that explains much of the observed dependence. The remaining dependence between the two observed variables $X, Y$ (which is unexplained by $Z$) is measured using conditional mutual information $I(X; Y|Z)$. The suitability of this metric stems from the fact that $I(X; Y|Z) = 0 \iff X \perp\!\!\!\!\perp Y | Z$. The smaller $Z$ makes $I(X; Y|Z)$, the more dependence it explains. While it is easy to construct a $Z$ that makes $I(X; Y|Z) = 0$, our goal is to discover a simple latent variable $Z$. To quantify the simplicity of the latent variable, we use its Shannon entropy $H(Z)$. Moreover, we would like to allow a tradeoff between these two factors, namely the simplicity of the latent variable and the residual dependency between $X, Y$ after conditioning on $Z$. Accordingly, we introduce the loss function

$$
\mathcal{L} = I(X; Y|Z) + \beta H(Z). 
$$

(1)

Recall in our setting that we have access of $p(x, y)$, the distribution between the discrete observed random variables $(X, Y)$ (with card$(X) = m$ and card$(Y) = n$). Thus, constructing a latent variable $Z$ is equivalent to constructing a joint distribution $q(x, y, z)$ between three variables $(X, Y, Z)$, that respects the observed joint between $(X, Y)$, i.e., $p(x, y)$. This leads to the requirement that $\sum_z q(x, y, z) = p(x, y)$. Rather than optimizing for $q(x, y, z)$ and forcing this constraint, we simply optimize for $q(z|x, y)$ and set $q(x, y, z) = q(z|x, y)p(x, y)$. Therefore we have $\mathcal{L} = \mathcal{L}(q(z|x, y))$.

Additionally, the cardinality of $Z$ is one measure of simplicity of $Z$, and further determines the number of variables we optimize to minimize the loss $\mathcal{L}$. If card$(Z) = k$, card$(X) = m$, card$(Y) = n$, to describe the conditional $q(z|x, y)$ we need $kmn$ non-negative numbers. Moreover, we have the constraint that $\sum_z q(z|x, y) = 1, \forall x, y$.

To this end, we propose *Algorithm LatentSearch* that starting with the known $p(x, y)$, iteratively computes $q(z|x, y)$ that optimizes to minimize the loss $\mathcal{L}$. Specifically, it marginalizes the joint $q_i(x, y, z)$ to get $q_i(z|x), q_i(z|x)$, and imposing a scaled product form on these marginals, updates the joint to return $q_{i+1}(x, y, z)$. This is formally shown in Algorithm 1. This decomposition and update is motivated by the partial derivatives associated with the Lagrangian of the loss function $\mathcal{L}$, and has the formal properties described below. The proofs are delegated to the supplementary material.

**Theorem 1.** The stationary points of LatentSearch are also the stationary points of the loss function in (1).

**Theorem 2.** For $\beta = 1$, LatentSearch converges to either a local minimum or a saddle point of the loss function in (1).
there does not exist a joint distribution where independently and uniformly randomly from the probability simplex in the appropriate dimensions, for such a \( Z \) distribution. However note that we do not observe a given graph, all but a measure zero set are faithful \cite{14}. Therefore, except for a measure zero set, \( X \perp \perp Y \mid Z \) for distributions from the triangle graph. However note that we do not observe \( Z \) and ask the question does there exist such a \( Z \)?

\[ \text{Algorithm 1 LatentSearch: Iterative Update Algorithm} \]

**Input:** Supports of \( x, y, z, X, Y, Z \), respectively and a parameter \( \beta > 0 \). Observed joint \( p(x, y) \). Initialization \( q_1(z|x, y) \). Number of iterations \( N \).

**Output:** Joint distribution \( q(x, y, z) \)

for \( i \in [N] \) do

Form the joint and marginalize:

\[
q_i(x, y, z) = \frac{\sum_{y \in Y} q_i(x, y, z)}{\sum_{y \in Y} q_i(x, y, z)} \quad q_i(z) = \sum_{x \in X, y \in Y} q_i(x, y, z) \quad q_i(y) = \sum_{x \in X, z \in Z} q_i(x, y, z)
\]

Update:

\[
q_{i+1}(z|x, y) = \frac{1}{N(x, y)} q_i(z|x) q_i(z|y) \quad N(x, y) = \sum_{z \in Z} q_i(z|x) q_i(z|y)
\]

end for

return \( q_{N+1}(z|x, y)p(x, y) \)

LatentSearch can be run a number of times by varying the value of \( \beta \) to discover what we believe is a fundamental \( I(X; Y \mid Z) \) vs \( H(Z) \) tradeoff curve. An example is given in Figure 3 in the supplementary material. We believe the algorithm finds an approximation to a fundamental tradeoff curve such that no point below this curve can be achieved for a given joint distribution \( p(x, y) \).

### 5 Detecting Spurious Correlations

Consider the two causal graphs given in Figure 1. Suppose there exists an algorithm that can answer the question "Is there a simple latent variable that can make \( X, Y \) conditionally independent?". Then we can use the such an algorithm to recover the true graph: If the answer is yes (i.e. there is a simple \( Z \) that renders \( (X, Y) \) to be conditionally independent), then declare the latent graph to be the true graph. If the answer is no, declare the triangle graph to be the true graph.

Now suppose that the joint distribution comes truly from the triangle graph, and we have access only to \( p(x, y) \). Then, if \( k > n \), it is possible to construct a latent graph that is indistinguishable from the triangle graph, i.e. agrees over the observed over \( p(x, y) \). This is trivially possible for instance by setting \( Z = X \) or \( Z = Y \). Below, we show that when \( k < \min\{m, n\} \), then for any random instance (construction detailed in Theorem 3) of the triangle graph\footnote{If \( (X, Y, Z) \) were fully observable, then it is known that among all distributions that are Markov with respect to a given graph, all but a measure zero set are faithful \cite{14}. Therefore, except for a measure zero set, \( X \perp \perp Y \mid Z \) for distributions from the triangle graph. However note that we do not observe \( Z \) and ask the question does there exist such a \( Z \)?} we cannot construct such a low-cardinality \( Z \) (equivalently, the simple test fails only on a measure zero set of joint distributions).

**Theorem 3.** Consider three discrete random variables \( X, Y, Z \) with supports \( [m], [n], [k] \), respectively, where \( k < \min\{m, n\} \). Let \( p(x, y, z) \) be the joint distribution over \( X, Y, Z \). Consider the following generative model for \( p(x, y, z) \): Let the conditional distributions \( p(Z), p(X|z), p(Y|x, z) \) be sampled independently and uniformly randomly from the probability simplex in the appropriate dimensions, for any realizations \( (z, x, y) \in [k] \times [m] \). Then, with probability 1, there does not exist any joint distribution \( q(x, y, z) \) such that \( \sum_z q(x, y, z) = p(x, y) \) and \( X \perp \perp Y \mid Z \).

**Corollary 1.** For almost all joint distributions that are obtained for triangle graph in Figure 1, there does not exist a joint distribution \( q(x, y, z) \) that can be encoded by the latent graph.
Proof. The statement follows from the fact that the proposed generative model induces a non-zero probability measure on every joint distribution, which is the set of distributions that can be encoded from the triangle graph and any distribution that can be encoded by the latent graph requires \( X \perp \perp Y \mid Z \), which we have shown happens with probability zero.

We expect a similar claim to hold, had we used Shannon entropy instead of cardinality. If true, this would allow us to consider latents with cardinality greater than \( n \), but with their Shannon entropy being small (formalized below). This can be implemented using LatentSearch (Algorithm 1) as a black box for recovering the simplest latent variable. The corresponding algorithm is given in Algorithm 2 (denoted henceforth as InferGraph).

Suppose the latent factor has \( n \) states, i.e., the same number of states as \( Y \). When the probability values are in general position in the sense described in Theorem 3 and the model comes from the triangle graph, we expect that no matter what the decomposition is, the latent variable’s entropy cannot be much less than the entropies of \( X,Y \). Motivated by this, we propose a conjecture that formalizes the claim that most of the joint distributions from the complete graph factorize only with latents with entropy close to \( \min\{H(X),H(Y)\} \).

Conjecture 1. Consider the following generative model for the joint distribution \( p(x,y) \) over two discrete variables \( X,Y \) with \( m,n \) states, respectively: Let the distribution of \( Z \) be sampled from Dirichlet(\( \alpha \)) for some \( \alpha \leq 1 \). Let each conditional distribution for the triangle graph, i.e., \( P(X\mid z), P(Y\mid x,z), \forall x,z \) be sampled with Dirichlet(1), i.e., uniformly from the simplex. Then there are constants \( a,b \) such that with probability 1, any joint distribution \( q(x,y,z) \) where \( \sum_z q(x,y,z) = p(x,y) \) and \( X \perp \perp Y \mid Z \) satisfies \( H(Z) \geq \theta = a \min\{H(X),H(Y)\} - b \).

Algorithm 2 InferGraph: Causal Inference Algorithm

Input: \( k \) : Cardinality of the latent variable \( Z \) to be constructed. Observed joint \( p(x,y) \) over the variables \( X,Y \). \( \theta \) : Threshold for \( H(Z) \). \( T \) : Conditional mutual information threshold.

Initialize a set of \( N \) conditional distributions \( q_i^0(z\mid x,y), i \in [N] \).

for \( i \in [N] \) do

\( q_i(z\mid x,y) \leftarrow \) LatentSearch (Algorithm 1) with input \( q_i^0(z\mid x,y) \).

Calculate \( I^i(X;Y\mid Z) \) and \( H^i(Z) \) from \( q_i^i(x,y,z) = q_i(z\mid x,y)p(x,y) \).

end for

\( S = \{i : I^i(X;Y\mid Z) \leq T\} \).

\( h = \min(\{H^i(Z) : i \in S\}) \)

if \( h > \theta \) then

\( D = X \leftarrow Z \rightarrow Y, X \rightarrow Y \)

else if \( h \leq \theta \) then

\( D = X \leftarrow Z \rightarrow Y \)

end if

return Causal Graph \( D \).

6 Simulations
6.1 Synthetic Data

In this section, our objective is to distinguish the two causal graphs given in Figure 1. Figure 2 shows how the recovered latent variable’s entropy varies with the entropy of the true latent variable,
As can be seen, thresholding at 
with probability very close to 1, supporting Conjecture 1.

As observed, there is a region of low-entropy latent variable regime for which 
LatentSearch can be used to distinguish between the two causal graphs with a properly chosen threshold, e.g., if the entropy of the true latent is less than 3 bits for \(|X| = |Y| = 20\).

As can be seen, thresholding at \(\min\{H(X), H(Y)\} - 1\) allows us to distinguish the two causal graph with probability very close to 1, supporting Conjecture 1. (b) \(P(\text{Est.: Latent}|\text{True: Latent})\). (c) \(P(\text{Est.: Complete}|\text{True: Complete})\). All thresholds perfectly classify the complete graphs, whereas latent graphs are accurately classified only for the threshold \(\theta = \min\{H(X), H(Y)\} - 1\).
when the causal graph is the latent graph shown in orange and the triangle graph (see Figure 1) shown in blue. The scatter plots are obtained for conditional mutual information threshold of 0.001: For each sampled causal model (each dot in the scatter plots), we randomly initialized 40 conditional distributions for different values of $\beta$ in $[0, 0.025]$ and run LatentSearch (Algorithm 1) for 1000 iterations. Each conditional distribution is chosen uniformly randomly from the corresponding simplex. After LatentSearch terminates, of all the 40 recovered distributions we picked the one with minimum entropy of all those that satisfy $I(X; Y|Z) \leq 0.001$. To obtain the scatter plots, for each causal graph, we repeated the above procedure 500 times for each graph, where each 125 of 500 samples are obtained from the Dirichlet distribution with parameters $[1.0, 0.5, 0.2, 0.1]$. This lets us induce a more uniform distribution on the entropy $H(Z)$ (hence the contiguity of samples in $x$ axis). Finally, for each point in the scatter plot, we predicted the causal graph: In this experiment, we assume we know the true upper bound on the maximum entropy of the latent variable and used this as the threshold for InferGraph (Algorithm 2). Figure 2(d) shows that when latent variable has cardinality less than $\min\{m, n\}$, we cannot find a latent that makes them (almost) conditionally independent. Therefore the InferGraph algorithm has almost perfect accuracy. In Figure 2(e) cardinality of the latent is chosen to be the same as the cardinality of $X, Y$. As observed, for entropy values less than 3.5 bits, classification is near perfect. When the cardinality of the latent variable is bigger than the cardinality of $X, Y$ (Figure 2(f)), accuracy goes down earlier, around 3 bits. This simulation illustrates that, if we know an upper bound on the entropy of the latent variable which is smaller than $\log(n)$, the InferGraph algorithm can be used to detect the true causal graph.

Next, to check the validity of our conjecture, we run InferGraph, where we set the threshold $\theta$ for the latent entropy as a function of $\min\{H(X), H(Y)\}$. The results are given in Figure 3. We observe that as $n$ is increased, accuracy goes to 1 for $\theta = \min\{H(X), H(Y)\} - 1$, whereas accuracy goes to 0 for $\theta = 2, \theta = 0.5 \min\{H(X), H(Y)\}$. This supports the hypothesis that $a = 1$ in Conjecture 1.

We compared our algorithm with gradient descent and NMF, which we outperform in terms of convergence and performance. We also apply EM algorithm to the output of LatentSearch and observe that EM does not help recover better solutions, in terms of $I(X; Y|Z), H(Z)$ trade-off. These results are given in the supplementary material in Section 8.5.

6.2 Causal Graph Skeleton Recovery on Adult Dataset

In this section, we study the Adult dataset from UCI Machine Learning Repository [5]. This dataset has 14 attributes 8 of which are discrete: workclass, education, marital status, occupation, relationship, race, sex, native country. It has 45222 samples (after dropping rows with missing values)\(^5\). The abundance of samples and small number of discrete states for these variables allows us to accurately estimate the joint probability distributions.

Our objective is to test the detection accuracy of InferGraph on a real causal graph. Since we are not given information about the latents on this graph, we assume there are no latents. We initialize with the complete undirected graph on the graph vertices. We apply our algorithm on every pair of observed variables $X, Y$ and estimate the joint distribution $p(x, y)$. We then run LatentSearch for 100 $\beta$ values linearly chosen in the range $[0, 0.025]$ for 1000 iterations for every $\beta$ value. Based on the obtained latent variable constructions, we find the minimum entropy the latent variable requires to make the conditional mutual information $I(X; Y|Z)$ less than 0.0005, which we call this $h_{\min}$. For each $X, Y$, we compare $h_{\min}$ with the threshold $\theta = 0.8 \min\{H(X), H(Y)\}$: If $h_{\min} < \theta$, we remove the edge $X \rightarrow Y$, else we keep it. After running this algorithm for every pair, we obtain an estimate of the graph skeleton. Our result is shown in Figure 4(a) along with the skeletons obtained.

\(^5\)Data requires mild cleaning: For example before cleanup, "United-states" and "united-states" are treated as different states for the native-country variable.
by hill-climbing algorithm that uses BIC score, shown in Figure 4(b), and the skeleton obtained via PC algorithm, shown in Figure 4(c). These structures are given in [13]. Surprisingly, our results are identical to the one recovered by hill-climbing algorithm except for a single edge. However, it should be noted that our algorithm is sensitive to the choices of both thresholds for $I(X; Y|Z)$ and entropy threshold $\theta$. For example, if we set $\theta = \min\{H(X), H(Y)\}$, we recover empty graph, whereas at least some of the edges are excepted to be direct from the context of the dataset. Setting this threshold based on a dataset is an interesting direction, which is left for future work.

Figure 4: Causal graph skeleton recovered by (a) our algorithm (InferGraph) for entropy threshold $\theta$ set to $\theta = 0.8 \min\{H(X), H(Y)\}$, (b) by hill-climbing algorithm with BIC score, (c) PC algorithm [13]. InferGraph can recover almost the same graph recovered by the hill-climbing algorithm with BIC score for this thresholding function for $\theta$.

7 Conclusion

In this paper, we study the problem of discovering a simple (discrete) random variable $Z$ that best explains the relationship between a pair of random variables $(X, Y)$. We formulate this through minimization of a loss function that trades off between entropy of $Z$ (the simple variable) and the conditional mutual information between $(X, Y)$ given $Z$. The resulting algorithm – LatentSearch – then is used to detect if a direct causal relation exists between $(X, Y)$ in the presence of a latent variable $Z$.

8 Appendix

8.1 $I(X; Y|Z)$ vs. $H(Z)$ Tradeoff Curve

Figure 5 shows the $I(X; Y|Z)-H(Z)$ tradeoff LatentSearch (Algorithm 1) obtains for a joint distribution sampled as follows: The distribution of $Z$ as well as the conditional distributions $p(X|z), p(Y|z), \forall z$ are chosen uniformly at random over the simplex.
Figure 5: $I(X; Y|Z)$ vs. $H(Z)$ tradeoff curve obtained by LatentSearch (Algorithm 1) for an arbitrary joint $p(x, y)$ from the graph $X \leftarrow Z \rightarrow Y$. We observed that the curve’s shape is consistent across many runs irrespective of the graph, although the crossing point where $I(X; Y|Z) = 0$ changes.

8.2 Proof of Theorem 1

We write the objective function more explicitly in terms of the optimization variables $q(z|x, y)$:

$$
\mathcal{L}(q(\cdot|\cdot, \cdot)) = \sum_{x, y, z} q(x, y, z) \log \left( \frac{q(x, y|z)}{q(x|z)q(y|z)} \right) - \beta \sum_{z} q(z) \log(q(z))
$$

$$
= \sum_{x, y, z} p(x, y)q(z|x, y) \log \left( \frac{q(z|x, y)}{q(z|x)q(z|y)} \right) + I(X; Y) + (1 - \beta) \sum_{z} q(z) \log(q(z)),
$$

by Bayes rule and assuming that $q(z|x, y)$ and $p(x, y)$ are strictly positive.

Our objective then is

$$
\text{minimize}_{q(z|x, y)} \mathcal{L}(q(z|x, y))
$$

subject to

$$
\sum_{z} q(z|x, y) = 1, \ \forall x, y,
$$

$$
q(z|x, y) \geq 0, \ \forall z, x, y.
$$

We can write the Lagrangian, which we represent with $\mathcal{L}$, as

$$
\mathcal{L} = \sum_{x, y, z} p(x, y)q(z|x, y) \log \left( \frac{q(z|x, y)}{q(z|x)q(z|y)} \right) + I(X; Y) + (1 - \beta) \sum_{z} q(z) \log(q(z))
$$

$$
+ \sum_{x, y} \delta_{x, y} \left( \sum_{z} q(z|x, y) - 1 \right)
$$

In order to find the stationary points of the loss, we take its first derivative and set it to zero. To compute the partial derivatives, notice that $q(z|x), q(z|y), q(z)$ are linear functions of $q(z|x, y)$ (use Bayes rule and marginalization). We can then easily write the partial derivatives of these quantities.
with respect to $q(z|x, y)$ as follows:

$$\frac{\partial q(z|x)}{\partial q(z|x, y)} = \frac{\partial \sum_{y'} q(z|x', y)p(y'|x)}{\partial q(z|x, y)} = p(y|x),$$

$$\frac{\partial q(z|y)}{\partial q(z|x, y)} = \frac{\partial \sum_{x'} q(z|x', y)p(x'|y)}{\partial q(z|x, y)} = p(x|y),$$

$$\frac{\partial q(z)}{\partial q(z|x, y)} = \frac{\partial \sum_{x', y'} q(z|x', y')p(x', y')}{\partial q(z|x, y)} = p(x, y).$$

Using these expressions we have the following.

$$\frac{\partial \mathcal{L}}{\partial q(z|x, y)} = p(x, y) \left[1 + \log(q(z|x, y)) - (1 + \log(q(z|x)))\right] - (1 + \log(q(z|y))) + (1 - \beta)(1 + \log(q(z))) + \delta_{x,y} \right]$$

$$= p(x, y) \left[-\beta + \delta_{x,y} + \log \left(\frac{q(z|x, y)q(z)^{1-\beta}}{q(z|x)q(z|y)}\right)\right]$$

Assuming $p(x, y) > 0$, any stationary point then satisfies

$$q(z|x, y) = \left(\frac{1}{2}\right)^{\beta - \delta_{x,y}} \frac{q(z)^{1-\beta}}{q(z|x)q(z|y)}. \quad (7)$$

Since $q(z|x, y)$ is a probability distribution, we have

$$\sum_z q(z|x, y) = \left(\frac{1}{2}\right)^{\beta - \delta_{x,y}} \sum_z q(z)^{1-\beta} = 1 \quad (8)$$

Defining $N(x, y) := \left(\frac{1}{2}\right)^{\beta - \delta_{x,y}}$, we have

$$N(x, y) = \frac{1}{\sum_z \frac{q(z)^{1-\beta}}{q(z|x)q(z|y)}}. \quad (9)$$

From the algorithm description, any stationary point of Algorithm 1 should satisfy

$$q(z|x, y) = \frac{1}{N(x, y)} \frac{q(z|x)q(z|y)}{q(z)^{1-\beta}}, \quad (10)$$

for the same $N(x, y)$ defined above. Therefore a point is a stationary point of the loss function if and only if it is a stationary point of LatentSearch (Algorithm 1).

8.3 Proof of Theorem 2

We can rewrite the loss as

$$\mathcal{L}(\cdot|\cdot) = \sum_{x,y,z} q(x, y, z) \log \left(\frac{q(x, y|z)}{q(x|z)q(y|z)}\right) - \beta \sum_z q(z) \log(q(z))$$

$$= \sum_{x,y,z} p(x, y)q(z|x, y) \log \left(\frac{q(z|x, y)}{q(z|x)q(z|y)}\right) + I(X; Y) + (1 - \beta) \sum_z q(z) \log(q(z)), \quad (11)$$

$$= \sum_{x,y,z} p(x, y)q(z|x, y) \log \left(\frac{q(z|x, y)}{q(z|x)q(z|y)}\right) + I(X; Y) + (1 - \beta) \sum_z q(z) \log(q(z)), \quad (12)$$
Algorithm 1.

To see that (15) is equivalent to (14), notice that the optimum for the inner minimization is $r^\ast(z|z) = q(z|x)$ and $s^\ast(z|x) = q(z|y)$. This is due to the fact that (15) is convex in $r(z|x)$ and $s(z|y)$ and concave in $t(z)$, which can be seen through the partial derivatives of the Lagrangian:

$$L(q(z|x), q(z|y)) = \sum_{x,y,z} p(x, y) q(z|x, y) \log \left( \frac{q(z|x, y)}{r(z|xs(z|y))} \right) + I(X; Y).$$

Our objective is

$$\begin{align*}
\text{minimize} & \quad L(q(z|x), q(z|y)) \\
\text{subject to} & \quad \sum_z q(z|x, y) = 1, \forall x, y.
\end{align*}$$

Notice that $L(q(z|x), q(z|y))$ is not convex or concave in $q(z|x, y)$. However we can rewrite the minimization as follows:

$$\begin{align*}
\text{minimize} & \quad \sum_{x,y,z} p(x, y) q(z|x, y) \log \left( \frac{q(z|x, y)}{r(z|xs(z|y))} \right) + I(X; Y) \\
\text{subject to} & \quad \sum_z q(z|x, y) = 1, \forall x, y \\
& \quad \sum_z r(z|x) = 1, \forall x, \\
& \quad \sum_z s(z|y) = 1, \forall y.
\end{align*}$$

To see that (15) is equivalent to (14), notice that the optimum for the inner minimization is $r^\ast(z|x) = q(z|x)$ and $s^\ast(z|x) = q(z|y)$. This is due to the fact that (15) is convex in $r(z|x)$ and $s(z|y)$ and concave in $t(z)$, which can be seen through the partial derivatives of the Lagrangian:

$$\begin{align*}
\text{minimize} & \quad \sum_{x,y,z} p(x, y) q(z|x, y) \log \left( \frac{q(z|x, y)}{r(z|xs(z|y))} \right) + I(X; Y) \\
& \quad + \sum_{x,y} \delta_{x,y} \left( \sum_z q(z|x, y) - 1 \right) + \sum_x \eta_x \left( \sum_z r(z|x) - 1 \right) \\
& \quad + \sum_x \nu_y \left( \sum_z s(z|y) - 1 \right)
\end{align*}$$

For fixed $q(z|x, y), s(z|y)$, we have

$$\frac{\partial \hat{\mathcal{L}}}{\partial r(z|x)} = -\frac{p(x)q(z|x)}{r(z|x)} + \eta_x$$

$$\frac{\partial^2 \hat{\mathcal{L}}}{\partial r(z|x)^2} = \frac{p(x)q(z|x)}{r(z|x)^2}.$$

Therefore $\hat{\mathcal{L}}$ is convex in $r(z|x)$ and the optimum can be obtained by setting the first derivative to zero. Then we have

$$r^\ast(z|x) = \frac{p(x)q(z|x)}{\eta_x}, \forall x, z.$$  

Since we have $\sum_z r^\ast(z|x) = \frac{b(x)}{\eta_x} \sum_z q(z|x) = 1$, we obtain $r^\ast(z|x) = q(z|x)$. Similarly, we can show that $s^\ast(z|x) = q(z|y)$. Notice that this inner minimization is exactly the same as the first update of Algorithm 1.
We can also show that $\mathcal{L}$ is convex in the variables $r, s$ jointly: This can be seen through the fact that
\[
\frac{\partial^2 \tilde{\mathcal{L}}}{\partial q(z|x,y)} = 0
\]
and the Hessian is positive definite.

This concludes that (15) is equivalent to (4). Moreover, since the objective function is convex in $q(z|x, y)$ and also jointly convex in $r(z|x), s(z|y)$, we can switch the order of the minimization terms. Therefore, we can equivalently write

\[
\begin{align*}
\text{minimize } & \quad \sum_{x,y,z} p(x,y; q(z|x,y)) q(z|x,y) \log \left( \frac{q(z|x,y)}{r(z|x)s(z|y)} \right) + I(X; Y) \\
\text{minimize } & \quad \sum_{x,y} \delta_{x,y} \left( \sum_{z} q(z|x,y) - 1 \right) + \sum_{x} \eta_{x} \left( \sum_{z} r(z|x) - 1 \right) \\
& \quad + \sum_{x} \nu_{y} \left( \sum_{z} s(z|y) - 1 \right)
\end{align*}
\]

Let us analyze the inner minimization in this equivalent formulation for fixed $r(z|x), s(z|y)$. Similarly, we can take the partial derivative as follows:

\[
\frac{\partial \tilde{\mathcal{L}}}{\partial q(z|x,y)} = p(x,y) \left[ 1 + \log(q(z|x,y)) - \log(r(z|x)) - \log(s(z|y)) + \delta_{x,y} \right]
\]

\[
= p(x,y) \left[ 1 + \delta_{x,y} + \log \left( \frac{q(z|x,y)}{r(z|x)s(z|y)} \right) \right]
\]

\[
\frac{\partial^2 \tilde{\mathcal{L}}}{\partial q(z|x,y)^2} = p(x,y) \left[ \frac{1}{q(z|x,y)} \right].
\]

Notice that $\frac{\partial^2 \tilde{\mathcal{L}}}{\partial q(z|x,y)^2} > 0$. Hence $\tilde{\mathcal{L}}$ is convex in $q(z|x,y)$. Then the optimum can be obtained by setting the first derivative to zero. We have

\[
p(x,y) \left[ 1 + \delta_{x,y} + \log \left( \frac{q(z|x,y)}{r(z|x)s(z|y)} \right) \right] = 0,
\]

or equivalently

\[
q(z|x,y) = \left( \frac{1}{2} \right)^{1+\delta_{x,y}} r(z|x)s(z|y).
\]

Note that if we define

\[
N(x, y) := \sum_{z} r(z|x)s(z|y),
\]

since $\sum_{z} q(z|x,y) = \left( \frac{1}{2} \right)^{1+\delta_{x,y}} \sum_{z} r(z|x)s(z|y) = 1$, we can write

\[
q(z|x,y) = \frac{1}{N(x,y)} r(z|x)s(z|y).
\]

This is exactly the same as the second update of LatentSearch (Algorithm 4) if $r(z|x) = q(z|x), s(z|y) = q(z|y)$.

Therefore, if $q_i(z|x, y)$ is the current conditional at iteration $i$, the next update of LatentSearch (Algorithm 4) is equivalent to first solving the inner minimization of (15) thereby assigning $r(z|x) = q_i(z|x), s(z|y) = q_i(z|y)$, then switching the order of the minimization operations, and solving the
inner minimization of (20), therefore assigning \( q_{i+1}(z|x,y) = \frac{1}{N(x,y)} q_i(z|x)q_i(z|y) \). In each of this two-step optimization iteration, either loss function goes down, or it does not change. If it does not change, the algorithm has converged. Otherwise, it cannot go down indefinitely since loss (1) is lower bounded as \( I(X;Y|Z) \geq 0 \) and \( H(Z) \geq 0 \) and therefore has to converge. This proves convergence of the algorithm to either a local minimum or a saddle point. The converged point cannot be a local maximum since it is arrived at after a minimization step.

\[ \square \]

8.4 Proof of Theorem 3

Since \( X, Y \) are discrete variables, we can represent the joint distribution of \( X, Y \) in matrix form. Let \( M = [p(x,y)](x,y)\in[m]\times[n] \). With a slight abuse of notation, let \( z := [z_1, z_2, \ldots, z_k] \) be the probability mass (row) vector of variable \( Z \), i.e., \( \mathbb{P}[Z = i] = z[i] = z_i \). Similarly, let \( x_z := [x_{z,1}, x_{z,2}, \ldots, x_{z,k}] \) be the conditional probability mass vector of \( X \) conditioned on \( Z = z \), i.e., \( \mathbb{P}[X = i|Z = z] = x_z[i] = x_{z,i} \). Finally, let \( y_{z,x} := [y_{z,x,1}, y_{z,x,2}, \ldots y_{z,x,n}] \) be the conditional probability mass vector of \( Y \) conditioned on \( X = x \) and \( Z = z \). We can write the matrix \( M \) as follows:

\[
M = \sum_{i=1}^{k} z_i \begin{bmatrix} x_{i,1}y_{i,1} \\ x_{i,2}y_{i,2} \\ \vdots \\ x_{i,m}y_{i,m} \end{bmatrix} \tag{26}
\]

Now suppose for the sake of contradiction that there exists such a \( q(x, y, z) \) such that \( \sum_z q(x, y, z) = p(x, y) \) and \( X \perp \!\!\!\!\!\!\perp Y | Z \). Then \( M \) admits a factorization of the form

\[
M = \sum_{i=1}^{k} z_i' \begin{bmatrix} x'_{i,1}y'_{i,1} \\ x'_{i,2}y'_{i,2} \\ \vdots \\ x'_{i,m}y'_{i,m} \end{bmatrix} \tag{27}
\]

where \( x'_{i,j}, y'_{i,j}, z'_i \) are due to the joint \( q(x, y, z) \) and are potentially different from their counterparts in (26). Notice that since \( X \perp \!\!\!\!\!\!\perp Y | Z \), we have \( y'_{i,j} = y'_{i,l}, \forall (j, l) \in [k] \times [m] \). Therefore the matrices

\[
\begin{bmatrix} x'_{i,1}y'_{i,1} \\ x'_{i,2}y'_{i,2} \\ \vdots \\ x'_{i,m}y'_{i,m} \end{bmatrix} \tag{28}
\]

are rank 1 \( \forall i \in [k] \). Therefore, \( M \) has NMF rank at most \( k \). Since matrix rank is upper bounded by the NMF rank, \( \text{rank}(M) \leq k \). Therefore, there exists a \( q(x, y, z) \) such that \( \sum_z q(x, y, z) = p(x, y) \) and \( X \perp \!\!\!\!\!\!\perp Y | Z \) only if \( \text{rank}(M) \leq k \). Next, we show that under the generative model described in the theorem statement, this happens with probability zero.

We have the following lemma:

**Lemma 1.** Let \( \{x_i : i \in [n]\} \) be a set of vectors sampled independently, uniformly randomly from the simplex \( S_{n-1} \) in \( n \) dimensions. Then, \( \{x_i : i \in [n]\} \) are linearly independent with probability 1.

**Proof.** If \( x_i \) are linearly dependent, then there exists a set \( \{\alpha_i : i \in [n]\} \) such that \( \sum_{i=1}^{n} \alpha_i x_i = 0 \). Let \( j = \text{arg max}\{i \in [n] : \alpha_i > 0\} \). Equivalently \( x_j \) is in the range of the set of vectors \( \{x_i : i \in [j-1]\} \).
Therefore, we can write
\[ \mathbb{P} \left\{ \{x_i : i \in [n]\} \right\} \text{ are linearly independent} \leq \sum_{i=2}^{n} \mathbb{P} \left\{ x_i \in R(x_1, \ldots, x_{i-1}) \right\}, \tag{29} \]
where \( R(x_1, \ldots, x_{i-1}) \), is the range of the vectors \( x_1, \ldots, x_{i-1} \), i.e., the vector space spanned by \( x_1, \ldots, x_{i-1} \).

Notice that \( \dim(R(x_1, \ldots, x_{i-1})) < n-1, \forall i \leq n-1 \). Therefore, the Lebesgue measure of \( R(x_1, \ldots, x_{i-1}) \cap S_{n-1} \) is zero with respect to the uniform measure over \( S_{n-1} \). Hence, \( \mathbb{P} \left\{ x_i \in R(x_1, \ldots, x_{i-1}) \right\} = 0, \forall i \leq n-1 \).

The above argument does not hold for the last term in the summation in (29). However, intersection of any \( n-1 \) dimensional vector space with the simplex \( S_{n-1} \) is an \( n-2 \) dimensional slice of the simplex \([19]\). Therefore, it has Lebesgue measure zero with respect to the uniform measure over the simplex.

**Corollary 2.** Let \( \{x_i : i \in [n]\} \) be a set of vectors sampled independently, uniformly randomly from the simplex \( S_{n-1} \) in \( n \) dimensions. Let \( \{c_i \neq 0 : i \in [n]\} \) be arbitrary real scalars that are non-zero. Then, \( \{c_i x_i : i \in [n]\} \) are linearly independent with probability 1.

**Proof.** The proof of Lemma [1] goes through since the span of a set of vectors does not change with scaling of the vectors.

\( \mathbf{M} \) is rank deficient if and only if its determinant is zero, i.e., \( \det(\mathbf{M}) = 0 \). The determinant is a polynomial in \( \{z_i : i \in [k]\} \). By induction, one can show that if a finite degree multivariate polynomial is not identically zero, the set of roots has zero Lebesgue measure (for example, see [3]).

The uniform measure over the simplex is absolutely continuous with respect to Lebesgue measure. Hence, the set of roots of a finite degree multivariate polynomial has measure zero with respect to the uniform measure over the simplex.

To show that \( \det(\mathbf{M}) \) is not identically zero, it is sufficient to choose a set of \( z_i 's \) for which determinant is non-zero. First, observe that by Corollary [2] each matrix
\[
\begin{bmatrix}
x_{i,1}y_{i,1} \\
x_{i,2}y_{i,2} \\
\vdots \\
x_{i,m}y_{i,m}
\end{bmatrix}
\tag{30}
\]
is full rank with probability 1. Let \( z_1 = 1 \) and \( z_j, \forall j \in \{2, 3, \ldots, k\} \). Then \( \det(\mathbf{M}) \neq 0 \) since \( \mathbf{M} \) is full rank. Therefore, the determinant, which is a polynomial in \( \{z_i : i \in [k]\} \) is not identically zero. This concludes the proof that with probability 1, \( \text{rank} (\mathbf{M}) = n > k \).

### 8.5 Comparing LatentSearch with EM, NMF and Gradient descent

#### 8.5.1 Comparison to gradient descent

We observed that iterative update step is slightly faster than the gradient descent step: Average time for iterative update: 0.000063 seconds. Average time for gradient update: 0.000078 seconds. More importantly, gradient descent takes much longer to converge and does not even achieve the same performance.
As observed in Figure 6, gradient descent converges only after 350000 iterations, whereas we observed that iterative update converges after around 200 iterations. Based on the average update times, this corresponds to a staggering difference of 0.01 seconds for the iterative algorithm vs. 27.3 seconds for the gradient descent algorithm. Although these results are for when \( n = m = k = 5 \) states, we observed single iterative update to be faster than single gradient update, giving similar performance comparison results for \( n = m = k = 80 \) states. A more detailed version is provided in Figure 9 in the Appendix.

The above result is for a constant step size of 0.001. With smaller step size, convergence slows down even further. With larger step size, gradient descent does not converge.

Figure 6: Comparison of the iterative algorithm with gradient descent. Blue points show the trajectory of gradient descent, whereas orange points show the trajectory for Algorithm 1 for 10 randomly initialized points with different \( \beta \) values in loss (1). Gradient descent takes 350,000 iterations to converge whereas iterative algorithm converges in about 200 iterations. Moreover, the points achieved by iterative algorithm are strictly better than gradient descent after convergence.

8.5.2 Comparison with EM algorithm

EM is the first algorithm suggested for solving the pLSA problem [7]. For the details of EM within this framework, please see [7]. However the EM algorithm for pLSA problem does not have any incentive to minimize the entropy of the latent factor.

In order to see how EM affects the entropy of the discovered latent variable, we run EM algorithm by initializing it at the points that are output by LatentSearch (Algorithm 1). Results are illustrated in Figure 7. We observe that the points obtained in the \( I - H \) plane migrate towards \( I(X;Y|Z) = 0 \) line, while staying above what we believe is a fundamental lower bound curve. We have not observed any improvement to our algorithm by this additional step, as it leads to increased entropy latent variables. For a more detailed illustration, please see Figure 10 in Appendix.

8.5.3 Comparison with NMF

Consider the joint distribution matrix \( \mathbf{M} \). Suppose we find an approximation to this matrix as \( \mathbf{M} \approx \mathbf{U} \mathbf{V} \) where the common dimension of \( \mathbf{U}, \mathbf{V} \) is \( k \) through NMF. This is equivalent to setting the dimension of the latent variable to \( k \). This can be seen as a hard entropy threshold on the entropy of the latent factor since \( H(Z) \leq \log(k) \). We can sweep through different dimensions and see how NMF performs compared to LatentSearch (Algorithm 1). Note that NMF is in general hard to solve. A commonly used approach is the iterative algorithm: Initialize \( \mathbf{U}_0, \mathbf{V}_0 \). Find the best \( \mathbf{U}_1 \) such that
Figure 7: Applying EM to the output of iterative algorithm migrates points to $I(X; Y|Z) = 0$ line: (a) Latent variables discovered by LatentSearch (Algorithm 1) shown on the $I(X; Y|Z) - H(Z)$ plane. (b,c) After applying EM algorithm on the points in (a) after 60 and 300 iterations. Observe that the points always remain above the line depicted by LatentSearch (Algorithm 1).

$M \approx U_1 V_0$. Then find the best $V_1$ such that $M \approx U_1 V_1$ and iterate. In the experiments, we used this iterative algorithm together with $l_1$ loss.

Figure 8: Comparison of the iterative algorithm to NMF for when $|X| = |Y| = 20, |Z| = 10$. When the true model comes from the causal graph $X \leftarrow Z \rightarrow Y$ in (a), iterative algorithm successfully finds latent variables that with entropy at most true latent entropy (shown as blue horizontal line), whereas NMF cannot achieve the same performance, irrespective of the dimension restriction to the latent variable. In (b) data comes from the causal model $X \leftarrow Z \rightarrow Y, X \rightarrow Y$. Although neither algorithm can identify a latent factor that makes $X, Y$ conditionally independent (vertical blue line), iterative algorithm finds strictly better latent factors in terms of both small entropy and conditional mutual information between $X, Y$.

8.6 Detailed Comparison with Gradient Descent

Figure 9 gives a more detailed comparison of Algorithm 1 to gradient descent.
Figure 9: A detailed version of Figure 6: Comparison of the iterative algorithm with gradient descent. Blue points show the trajectory of gradient descent, whereas orange points show the trajectory for Algorithm 1 for 10 randomly initialized points with different $\beta$ values in loss (1). Gradient descent takes 350,000 iterations to converge whereas iterative algorithm converges in about 200 iterations (not shown). Moreover, the points achieved by iterative algorithm are strictly better than gradient descent after convergence.

8.7 Detailed Results of Applying EM to the output of LatentSearch (Algorithm 1)

Figure 10 gives a more detailed description of the effect of applying EM to the output points of LatentSearch (Algorithm 1).
8.8 Entropy Thresholds Recovered by Algorithm 2 for Adult Dataset

In the following table, for every pair of observed variables $X, Y$ from the Adult dataset, we provide the minimum $H(Z)$ such that $X \perp \perp Y \mid Z$. Marginal entropies of each the variables are replicated in each row for ease of parsing. Please see the main text for a description of how the threshold and marginal entropies are used to infer the graph skeleton.
| relationship - race | Threshold | education | marital-status | native-country | occupation | race | relationship | sex | workclass |
|---------------------|-----------|-----------|----------------|----------------|------------|-----|--------------|-----|-----------|
| 0.298388229345      | 2.916     | 1.823     | 0.822          | 3.401          | 0.773      | 2.137| 0.91         | 1.42|
| sex - native-country| 0.5593792327 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| workclass - relationship | 0.647899328859 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| marital-status - race | 0.317382604528 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| education - sex | 0.44256193021 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| marital-status - native-country | 0.318245274335 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| education - native-country | 0.695226536202 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| occupation - race | 0.360543510539 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| workclass - native-country | 0.354718901671 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| race - native-country | 0.728427779233 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| relationship - native-country | 0.607195078663 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| marital-status - relationship | 1.53530463096 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| occupation - relationship | 1.45550458486 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| workclass - sex | 0.472765324227 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| marital-status - occupation | 1.24965445645 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| occupation - sex | 0.863184087645 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
| education - relationship | 1.39010810973 | 2.916 | 1.823 | 0.822 | 3.401 | 0.773 | 2.137 | 0.91 | 1.42 |
|                        | education - occupation | workclass - marital-status | workclass - race | education - race | workclass - education | race - sex | occupation - native-country | workclass - occupation | marital-status - sex | relationship - sex | education - marital-status |
|------------------------|------------------------|---------------------------|-----------------|-----------------|---------------------|-----------|---------------------------|----------------------|-------------------|-----------------|-------------------------|
| education - occupation | 2.26471544592          | 0.498648032438            | 0.43924357958   | 0.483681718567  | 1.0703086375        | 0.167841023602 | 0.665917280708               | 1.28023674998        | 0.802797928063    | 0.909648660891    | 1.13046716861             |
| workclass - marital-status | 2.916                 | 2.916                     | 2.916           | 2.916           | 2.916               | 2.916       | 2.916                      | 2.916                | 2.916             | 2.916           | 2.916                   |
| workclass - race       | 1.823                  | 1.823                     | 1.823           | 1.823           | 1.823               | 1.823       | 1.823                      | 1.823                | 1.823             | 1.823           | 1.823                   |
| education - race       | 0.822                  | 0.822                     | 0.822           | 0.822           | 0.822               | 0.822       | 0.822                      | 0.822                | 0.822             | 0.822           | 0.822                   |
| workclass - education  | 3.401                  | 3.401                     | 3.401           | 3.401           | 3.401               | 3.401       | 3.401                      | 3.401                | 3.401             | 3.401           | 3.401                   |
| marital-status - sex   | 0.773                  | 0.773                     | 0.773           | 0.773           | 0.773               | 0.773       | 0.773                      | 0.773                | 0.773             | 0.773           | 0.773                   |
| relationship - sex     | 2.137                  | 2.137                     | 2.137           | 2.137           | 2.137               | 2.137       | 2.137                      | 2.137                | 2.137             | 2.137           | 2.137                   |
| education - marital-status | 0.91                   | 0.91                      | 0.91            | 0.91            | 0.91                | 0.91        | 0.91                       | 0.91                 | 0.91              | 0.91            | 0.91                    |
| workclass - occupation | 1.42                   | 1.42                      | 1.42            | 1.42            | 1.42                | 1.42        | 1.42                       | 1.42                 | 1.42              | 1.42            | 1.42                    |
Figure 10: A detailed version of Figure 7. Applying EM to the output of iterative algorithm migrates points to $I(X; Y | Z = 0)$ line. Observe that the points always remain above the line depicted by LatentSearch (Algorithm 1).
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