Learning Structured Latent Factors from Dependent Data: 
A Generative Model Framework from Information-Theoretic Perspective

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Abstract

Learning controllable and generalizable representation of multivariate data with desired structural properties remains a fundamental problem in machine learning. In this paper, we present a novel framework for learning generative models with various underlying structures in the latent space. We represent the inductive bias in the form of mask variables to model the dependency structure in the graphical model and extend the theory of multivariate information bottleneck (Friedman et al., 2001) to enforce it. Our model provides a principled approach to learn a set of semantically meaningful latent factors that reflect various types of desired structures like capturing correlation or encoding invariance, while also offering the flexibility to automatically estimate the dependency structure from data. We show that our framework unifies many existing generative models and can be applied to a variety of tasks, including multi-modal data modeling, algorithmic fairness, and out-of-distribution generalization.

1. Introduction

Learning structured latent representation of multivariate data is a fundamental problem in machine learning. Many latent variable generative models have been proposed to date based on different inductive biases that reflect the model’s assumptions or people’s domain knowledge. For instance, the objectives of the family of $\beta$-VAEs (Higgins et al., 2016; Chen et al., 2018; Kim & Mnih, 2018) try to enforce a coordinate-wise independent structure among latent variables to discover disentangled factors of variations. While these methods have been proven useful in the field of applications on which they were evaluated, most of them are built-in rather heuristic ways to encode the desired structure. One usually needs to construct an entirely different model whenever the domain of application changes. In general, the type of inductive bias differs significantly across different applications. It is a burden to craft a different architecture for each application, and there have not been many studies done for the general and unified way of explicitly representing an inductive bias to be enforced in generative models.

In this paper, we propose a framework of generative model that can represent various types of inductive biases in the form of Bayesian networks. Our method can not only unify many existing generative models in previous studies, but it also can lead to new insights about establishing connections between different models across different domains and extending them to new applications.

We summarize our contributions in this work as: (i) We propose a novel general framework of probabilistic generative model with explicit dependency structure representation to learn structured latent representation of multivariate data. (ii) We propose an information-theoretic training objective by generalizing the multivariate information bottleneck theory to encode prior knowledge or impose inductive bias. (Sec. 3.3) (iii) We propose a flexible and tractable inference model with linear number of inference networks coupled with super-exponential number of possible dependency structures to model exponential number of inference distributions. (Sec. 3.4) (iv) We show that our proposed framework unifies many existing models and demonstrate its effectiveness in different application tasks, including multi-modal data generative modeling, algorithmic fairness, and out-of-distribution generalization.

2. Background

2.1. Notations

We use capital letters (i.e. $X \equiv X_{1:N}$) to denote a vector of $N$ random variables, and lower case letters (i.e. $x$) for the values. We use $P(X)$ to denote the probability distribution and corresponding density with $p(x)$. Given a set $S \subseteq \{1, 2, \ldots, N\}$ of indexes, we use $X^S \equiv [X_{i}\in S]$ to represent corresponding subset of random variables. Similar notation is used for binary indicator vector $b$ that $X^b \equiv [X_{i}\in b]$. 

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2.2. Probability and information theory

A Bayesian network $\mathcal{G} \equiv (\mathcal{V}, \mathcal{E})$ defined over random variables $X$ is a directed acyclic graph, consisting of a set of nodes $\mathcal{V} \equiv \{X_i\}_{i=1}^N$ and a set of directed edges $\mathcal{E} \subseteq \mathcal{V}^2$. A node $u$ is called a parent of $v$ if $(v, u) \in \mathcal{E}$, and for each random variable $X_i$, the set of parents of $X_i$ is denoted by $\text{Pa}^\mathcal{G}_i$. We use $\mathcal{G}^0$ to denote an empty Bayesian network $\mathcal{G}^0 \equiv (\mathcal{V}, \emptyset)$. If a distribution $P(X)$ is consistent with a Bayesian network $\mathcal{G}$, then it can be factorized as $p(x) = \prod_{i} p(x_i | \text{Pa}^\mathcal{G}_i)$, denoted by $p \equiv \mathcal{G}$.

We then briefly introduce the information theory concepts used in this paper here. The Shannon Entropy is defined as $H(X) = -\mathbb{E}_{p(x)} \log p(x)$ to measure the average number of bits needed to encode values of $X \sim P(X)$. The Kullback–Leibler Divergence (KLD) is one of the most fundamental distance between probability distributions defined as $D_{\text{KL}}(P \parallel Q) = \mathbb{E}_p \log \frac{p}{q}$. Mutual Information $I(X; Y)$ quantifies the mutual dependence between two random variables $X$ and $Y$. The mutual information is zero if and only if $X$ and $Y$ are independent.

Multi-Information is one of multivariable mutual information defined as $I(X_1, \ldots, X_N) = D_{\text{KL}}(p(x_1, \ldots, x_N) \parallel \prod_{i=1}^N p(x_i))$, which generalizes the mutual information concept to quantify the multivariate statistical independence for arbitrary number of random variables. (Lin. 1991) proposed a generalized Jensen-Shannon divergence defined as $D_{\text{JS}} = \sum_{i=1}^N \pi_i H(P_i) - \sum_{i=1}^N \pi_i H(P_i) = \mathbb{E}_p \log \frac{p}{q}$.

As shown in (Friedman et al., 2001), a variational autoencoder (VAE) (Kingma & Welling, 2014) is a probabilistic latent variable generative model $p_{\theta}(x | z) = p_{\theta}(z)p_{\theta}(x | z)$, where $p_{\theta}(z)$ is the prior of latent variables $Z$ and $p_{\theta}(x | z)$ is the likelihood distribution for observed variable $X$. The generative model is often optimized together with a tractable distribution $q_{\phi}(z | x)$ that approximates the posterior distribution. The distributions are usually parametrized by neural networks with parameters $\theta$ and $\phi$. The inference model and generation model are jointly optimized by a lower-bound of the KLD between $q_{\phi}$ and $p_{\theta}$ in the augmented space $(X, Z)$, namely ELBO:

$$\mathbb{E}_{q_{\phi}} \log p_{\theta}(x | z) - \mathbb{E}_{q_{\phi}(x)} D_{\text{KL}}(q_{\phi}(z | x) \parallel p_{\theta}(z)) \equiv \mathcal{L}_{\text{ELBO}}$$

(2)

Note $-\mathcal{L}_{\text{ELBO}} \geq D_{\text{KL}}(q_{\phi}(x) q_{\phi}(z | x) \parallel p_{\theta}(z) p_{\theta}(x | z))$ where $q_{\phi}(x) = p_{\text{data}}(x)$ denotes the empirical data distribution. The above objective can be optimized efficiently with the re-parametrization trick (Kingma & Welling, 2014; 2019).

2.4. Multivariate information bottleneck

Multivariate Information Bottleneck (MIB) theory proposed by (Friedman et al., 2001; Slonim et al., 2006) extends the information bottleneck theory (Tishby et al., 2000) to multivariate setting. Given a set of observed variable $X$, MIB framework introduced a Bayesian network $\mathcal{G}^{\text{in}}$ to define the solution space of latent variables $Z$ as $q(X, Z) \equiv \mathcal{G}^{\text{in}}$. Another Bayesian network $\mathcal{G}^{\text{out}}$ is introduced to specify the relevant information to be preserved in $Z$. Then the MIB functional objective is defined as $\mathcal{L}^1_{\text{MIB}}(q) = \mathcal{L}^{\text{in}}_{\phi}(X) - \beta \mathcal{L}^{\text{out}}_{\phi}(X)$. An alternative structural MIB functional objective is defined as $\mathcal{L}^2_{\text{MIB}}(q) = \mathcal{L}^{\text{in}}_{\phi}(X) + \gamma \mathbb{D}(q(x, z) \parallel \mathcal{G}^{\text{out}})$, and further relaxed by (Elidan & Friedman, 2005) as $\mathcal{L}^2_{\text{MIB}}(q, p) = \mathcal{L}^{\text{in}}_{\phi}(X) + \gamma D_{\text{KL}}(q(x, z) \parallel p(x, z))$. We refer to (Friedman et al., 2001; Elidan & Friedman, 2005) for more details of MIB theory.

3. Framework

3.1. Preliminaries

Given a dataset $\mathcal{D} = \{x^{(d)}\}_{d=1}^{D}$, we assume that observations are generated from some random process governed by a set of latent factors, which could be categorized into two types: private latent factors $U \equiv U_1, U_2, \ldots, U_N$ and common latent factors $Z \equiv Z_1, Z_2, \ldots, Z_M$. We use $U_i$ to denote the latent factors that are exclusive
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to the variable $x_i$ and assume a jointly independent prior distribution $P(U)$. We use $Z$ to denote the latent factors that are possibly shared by some subset of observed variables and assume a prior distribution $P(Z)$. The dimension of each $U_i$ and $Z_j$ is arbitrary.

3.2. Generative model with explicit dependency structure representation

**Generation model** We explicitly model the dependency structure from $Z$ to $X$ in the random generation process with a binary matrix variable $M^p = \{M^p_{ij}\} \in \{0, 1\}^{N \times M^p}$. $M^p_{ij} = 1$ when the latent factor $Z_j$ contributes to the random generation process of $X_i$, or otherwise $M^p_{ij} = 0$. Let $M_i^p = [M^p_{i1}, M^p_{i2}, \ldots, M^p_{iM^p}]$ denote the $i$-th row of $M$. We can define our generative model $p_\theta(x, z, u)$ as

$$ p_\theta(x, z, u) = p_\theta(z) \prod_{i=1}^N p_\theta(u_i) \prod_{i=1}^N p_\theta(x_i | z^{m^p_i}, u_i) $$

where $\theta$ is the parameter for parameterizing the generative model distribution. The structure of the generative model is illustrated by Bayesian network $G^p_{full}$ in Figure 2, where the structural variable $M^p$ is depicted as the dashed arrows.

**Inference** We introduce an inference model to approximate the true posterior distributions. We introduce another binary matrix variable $M^q = \{M^q_{ij}\} \in \{0, 1\}^{N \times M^q}$. $M^q_{ij} = 1$ when the observed variable $X_i$ contributes to the inference process of $Z_j$, or otherwise $M^q_{ij} = 0$. Let $M_i^q = [M^q_{i1}, M^q_{i2}, \ldots, M^q_{iM^q}]$ denote the $j$-th column of $M^q$. We assume that latent variables are conditionally jointly independent given observed variables. Then we can define our inference model $q_\phi(x, z, u)$ as:

$$ q_\phi(x, z, u) = q_\phi(z) \prod_{i=1}^N q_\phi(u_i | x_i) \prod_{j=1}^M q_\phi(z_j | x^{m^q_j}) $$

where $\phi$ is the parameter for parameterizing the inference distribution. The structure of the inference model is illustrated by Bayesian network $G^q_{full}$ in Figure 2, where the structural variable $M^q$ is depicted as the dashed arrows.

3.3. Learning from information-theoretic perspective

We motivate our learning objective based on the MIB (Friedman et al., 2001) theory. We can define a Bayesian network $G^q \equiv (\mathcal{V}^q, \mathcal{E}^q)$ that is consistent with the inference model distribution $q_\phi(x, z, u) = G^q$ according to $M^q$. A directed edge from $X_i$ to $U_i$ is added for each $i \in \{1, 2, \ldots, N\}$ and an edge from $X_i$ to $Z_j$ is added if and only if $m^q_{ij} = 1$. Note that we could omit all edges between observed variables in $G^q$ as shown in (Friedman et al., 2001; Elidan & Friedman, 2005). A Bayesian network $G^p \equiv (\mathcal{V}^p, \mathcal{E}^p)$ can be constructed according to $M^p$ in a similar way. As introduced in Eq. 2.4, we have the following structural variational objective from the MIB theory:

$$ \min_{p_\theta = G^p, q_\phi = G^q} \mathcal{L}(\theta, \phi) = \mathcal{I}_q^{G^q} + \gamma \mathcal{D}_{KL}(q_\phi \parallel p_\theta) $$

The above objective provides a principled way to trade-off between (i) the compactness of learned latent representation measured by $\mathcal{I}_q^{G^q}$, and (ii) the consistency between $q_\phi(x, z, u)$ and $p_\theta(x, z, u)$ measured by the KLD, through $\gamma > 0$.

We further generalize this objective to enable encoding a broader class of prior knowledge or desired structures into the latent space. We prescribe the dependency structure and conditional independence rules that the learned joint distribution of $(x, z, u)$ should follow, in the form of a set of Bayesian networks $\{G^k \equiv (\mathcal{V}^k, \mathcal{E}^k)\}, k = 1, \ldots, K$. We optimize over the inference distributions $q_\phi$ to make it as consistent with $G^k$ as possible, measured by its M-projection to $G^k$. Formally we have the following constrained optimization objective:

$$ \min_{p_\theta = G^p, q_\phi = G^q} \mathcal{L}(\theta, \phi) = \mathcal{D}_{KL}(q_\phi \parallel p_\theta) $$

s.t. $\mathbb{D}(q_\phi \parallel G^k) = 0 \quad k = 1, 2, \ldots, K$

In this way, we impose the preferences over the structure of learned distributions as explicit constraints. We relax the above constrained optimization objective with generalized Lagrangian

$$ \max_{\beta \geq 0} \min_{p_\theta = G^p, q_\phi = G^q} \mathcal{L} = \mathcal{D}_{KL}(q_\phi \parallel p_\theta) + \sum_{k=1}^K \beta_k \mathbb{D}(q_\phi \parallel G^k) $$

where $\beta \equiv [\beta_1, \beta_2, \ldots, \beta_K]$ is the vector of Lagrangian multipliers. In this work we fix $\beta$ as constant hyper-parameters, governing the trade-off between structural regularization and distribution consistency matching. Following the idea proposed in (Zhao et al., 2018), we could also generalize the distribution matching loss by using a vector of $T$ cost functions $\mathcal{C} = [C_1, C_2, \ldots, C_T]$ and a vector of Lagrangian multipliers $\alpha \equiv [\alpha_1, \alpha_2, \ldots, \alpha_T]$. Each $C_i$ can be any probability distribution divergence between $q_\phi$ and $p_\theta$, or any measurable cost function defined over corresponding samples. Thus we could decompose the overall objective as

$$ \mathcal{L} = \mathcal{L}_{\text{dist}} + \mathcal{L}_{\text{str_reg}} $$

$$ \mathcal{L}_{\text{dist}} = \sum_{i=1}^T \alpha_i C_i(q_\phi \parallel p_\theta), \quad \alpha \geq 0 $$

$$ \mathcal{L}_{\text{str_reg}} = \sum_{k=1}^K \beta_k \mathbb{D}(q_\phi \parallel G^k), \quad \beta \geq 0 $$

By setting $C_1 = \mathcal{D}_{KL}(q_\phi \parallel p_\theta)$ and $G^1 = G^q$, we can obtain that the original MIB structural variational objective
in Eq. 5 as a special case. We include the detailed proof in Appendix. A.1.

3.4. Tractable inference and generation

Though we have our generation and inference model defined in Sec. 3.2, it’s not clear yet how we practically parametrize \( q_\theta \) and \( p_\theta \) in a tractable and flexible way, to handle super-exponential number of possible structures \( M^p, M^q \) and efficient inference and optimization.

**Inference model** We identify the key desiderata of our inference model defined in Eq. 4 as (i) being compatible with any valid structure variable \( M^q \) and (ii) being able to handle missing observed variables in \( q(z_j \mid x^{m_j}) \), in an unified and principled way. Building upon the assumption of our generation model distribution \( p_\theta \) in Eq. 3 that all observed variables \( X \) are conditional jointly independent given \( Z \), we have following factorized formulation in the true posterior distribution \( p_\theta(z \mid x) \) by applying Bayes’ rule:

\[
p_\theta(z \mid x^S) = \frac{p_\theta(x^S \mid z)q_\theta(z)}{p_\theta(x^S)} = \frac{p_\theta(z)}{p_\theta(x^S)} \prod_{i \in S} p_\theta(x_i \mid z)
\]

\[
= \frac{p_\theta(z)}{p_\theta(x^S)} \prod_{i \in S} \frac{p_\theta(z \mid x_i)p_\theta(x_i)}{p_\theta(z)} \propto p_\theta(z) \prod_{i \in S} \frac{p_\theta(z \mid x_i)}{p_\theta(z)}
\]

(9)

where \( S \subseteq \{1, 2, \ldots, N\} \). In this way, we established the relationship between the joint posterior distribution \( p_\theta(z \mid x) \) and the individual posterior distribution \( p_\theta(z \mid x_i) \). We adopt the same formulation in our inference model distribution as \( q_\theta(z \mid x^S) \propto p_\theta(z) \prod_{i \in S} q_\theta(z \mid x_i) \), using \( N \) individual approximate posterior distributions \( q_\theta(z \mid x_i) \). In this work, we assume that \( p_\theta(z) \) and \( q_\theta(z \mid x_i) \) are all following factorized Gaussian distributions. And each individual posterior \( q_\theta(z \mid x_i) \) can be represented as:

\[
q_\theta(z \mid x_i) = \prod_{j=1}^M q_\theta(z_j \mid x_i)^m_j \propto p_\theta(z_j)^{1-m_j}
\]

(10)

where each \( q_\theta(z_j \mid x_i) \) is a multiplicative mixture between the approximated posterior \( q_\theta(z_j \mid x_i) \) and the prior \( p_\theta(z_j) \), weighted by \( m_j \). Since the quotient of two Gaussian distributions is also a Gaussian under well-defined conditions, we could parametrize the quotient \( \frac{q_\theta(z \mid x)}{p_\theta(z)} \) using a Gaussian distribution parametrized by \( \tilde{q}_\theta(z \mid x_i) \). In this case

\[
\frac{q_\theta(z \mid x_i)}{p_\theta(z)} = \prod_{j=1}^M \frac{q_\theta(z_j \mid x_i)^{m_j}p_\theta(z_j)^{1-m_j}}{p_\theta(z)^{m_j+1-m_j}} = \prod_{j=1}^M \left( \frac{\tilde{q}_\theta(z_j \mid x_i)}{p_\theta(z_j)} \right)^{m_j}
\]

(11)

where we use a inference network \( \tilde{q}_\theta(z_j \mid x_i) \) to parametrize \( q_\theta(z_j \mid x_i) = \tilde{q}_\theta(z_j \mid x_i) \).

We show our full inference distribution \( q_\theta(z \mid x) \) as:

\[
q_\theta(z \mid x^S) \propto \prod_{j=1}^M \left( \frac{p_\theta(z_j)}{\prod_{i \in S} (\tilde{q}_\theta(z_j \mid x_i))^{m_j}} \right)
\]

(12)

which is a weighted product-of-experts (Hinton, 2002) distribution for each latent variable \( Z_j \). We include the detailed derivation in Appendix. A.1. The structure variable \( M^q_j \) controls the weight of each multiplicative component \( \tilde{q}_\theta(z_j \mid x_i) \) in the process of shaping the joint posterior distribution \( q_\theta(z \mid x) \).

As a result of the Gaussian assumptions, the weighted product-of-experts distribution above has a closed-form solution. Suppose \( p_\theta(z) \sim \mathcal{N}(\mu_\theta, \sigma_\theta) \), \( \tilde{q}_\theta(z \mid x_i) \sim \mathcal{N}(\mu_i, \sigma_i) \). We produce “dummy” variables in \( m^q \), with \( m^q_i = 1 \) for all \( j \).

Then we have

\[
q_\theta(z \mid x^S) \sim \mathcal{N}(\mu^q, \sigma^q)
\]

(13)

With the derived inference model above, we are now able to model \( 2^N \) posterior inference distributions \( q_\theta(z \mid x^S) \forall S \), coupled with \( 2^N \times M \) possible discrete structures \( M^q \), with \( N \) inference networks \( \tilde{q}_\theta(z \mid x_i) \). Note that the introduced distribution \( q_\theta(z \mid x) \) remains valid when we extend the value of structure variable \( M^q \) to continuous domain \( \mathbb{R}^N \times M \), which paves the way to gradient-based structure learning.

**Generation model** We could parametrize our generation model \( p_\theta \) in a symmetric way using the weighted product-of-expert distributions using \( p_\theta(x_i \mid z_j) \) and \( M^p \). In this work we adopt an alternative approach, due to the consideration that the Gaussian distribution assumption is inappropriate in complex raw data domain, like image pixels. We instead use \( M^p \) as a gating variable and parametrize \( p_\theta(x_i \mid z^m_i) \) in the form of \( p_\theta(x_i \mid z^m_i) = p_\theta(x_i \mid z \circ m^p_i) \), where \( \circ \) denotes element-wise multiplication. We can see that it’s still tractable since the prior \( p_\theta(z) \) is known.

3.5. Tractable optimization

**Structural regularization** \( L_{\text{str-reg}} \) Let’s take a close look at the structural regularization term \( L_{\text{str-reg}} \) in our training objective Eq. 8. As introduced in Sec.2.4, we have \( D(\theta_\phi \parallel \theta^k) = \sum_{v \in \{x, z\}} I_q(v \mid p_\phi^O(v) = \sum_{v \in \{x, z\}} I_q(v \mid p_\phi^D(v)) \). This objective poses new challenge to estimate and optimize mutual information. Note that any differentiable mutual information estimations and optimization methods can be applied here. In this paper, we propose to use tractable variational lower/upper-bounds of the intractable mutual information by re-using distributions \( q_\theta \) and \( p_\theta \). We refer to (Poole et al., 2019) for a detailed
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Algorithm 1 Training with optional structure learning

Require: dataset $D = \{x^d\}_{d=1}^{D}$
Require: parameters $\phi, \theta, \rho^q, \rho^p$
Require: Bayesian Networks $\{\mathcal{G}^k = (\mathcal{V}^k, \mathcal{E}^k)\}$
Require: hyper-parameters $\alpha, \beta$
Require: number of iterations to update distribution parameters $\text{steps\_dist} > 0$
Require: number of iterations to update structure parameters $\text{steps\_str} \geq 0$
Require: mini-batch size $bs$
Require: gradient-based optimizer $\text{opt}$
initialize all parameters $\phi, \theta, \rho^q, \rho^p$
repeat
  for $step = 1$ to $\text{steps\_dist}$ do
    randomly sample a mini-batch $B$ of size $bs$ from dataset $D$
    evaluate loss $L_{\text{dist}}^B$ using Eq. 8
    compute gradients $\nabla_{\phi} L_{\text{dist}}^B, \nabla_{\theta} L_{\text{dist}}^B$
    $\text{opt}.\text{optimize}((\phi, \theta), [\nabla_{\phi} L_{\text{dist}}^B, \nabla_{\theta} L_{\text{dist}}^B])$
  end for
  for $step = 1$ to $\text{steps\_str}$ do
    randomly sample a mini-batch $B$ of size $bs$ from dataset $D$
    evaluate loss $L_{\text{score}}^B$ using Eq. 15
    compute gradients $\nabla_{\rho^q} L_{\text{score}}^B, \nabla_{\rho^p} L_{\text{score}}^B$
    $\text{opt}.\text{optimize}((\rho^q, \rho^p), [\nabla_{\rho^q} L_{\text{score}}^B, \nabla_{\rho^p} L_{\text{score}}^B])$
  end for
until converged

Distribution consistency $L_{\text{dist}}$ We aim to achieve the consistency between the joint distribution $q_{\phi}(x, z, u)$ and $p_{\theta}(x, z, u)$ through $T$ cost functions in $L_{\text{dist}}$. With the proposed inference model in Sec. 3.4, we could decompose our $L_{\text{dist}}$ into two primary components: (i) Enforcing $q_{\phi}(x, z, u) = p_{\theta}(x, z, u)$ Many previous works (Kingma & Welling, 2014; Tolstikhin et al., 2018; Dumoulin et al., 2017; Donahue et al., 2017) have been proposed to learn a latent variable generative model to model the joint distribution, any tractable objective can be utilized here, we adopt the ELBO as the default choice. (ii) Enforcing $q_{\phi}(z) = p_{\theta}(z)$ The reason that we explicitly include this objective in $L_{\text{dist}}$ is due to our $p_{\theta}$-dependent parametrization of $q_{\phi}(z | x) \propto p_{\theta}(z) \prod_{t=1}^{N} q_{\phi}(x_t | z)$. Thus we explicitly enforce the consistency between the induced marginal distribution $q_{\phi}(z) \equiv \mathbb{E}_{z \sim q_{\phi}(z | x)} p_{\theta}(z)$. Tractable divergence estimators for minimizing $C_T (q_{\phi}(z) \parallel p_{\theta}(z))$

Table 1. Distribution consistency objectives $L_{\text{dist}}$

| $C$ | definition |
|-----|------------|
| $C_0(x, z, u)$ | $D_{KL}(q_{\phi} \| p_{\theta})$ |
| $C_1(x, u)$ | $-L_{\text{ELBO}}(q_{\phi}(x, u), p_{\theta}(x, u))$ |
| $C_2(z)$ | $D_{\text{JS}}(q_{\phi}(z) \parallel p_{\theta}(z))$ |
| $C_{3i}(z)$ | $D_{KL}(q_{\phi}(z) \parallel p_{\theta}(z))$ |
| $C_4(x, z)$ | $D_{KL}(q_{\phi}(x, z) \parallel p_{\theta}(x, z))$ |

have been proposed and analyzed in previous works,

$$L_{\text{dist}} = \sum_{t=1}^{T-1} \alpha_t C_t(q_{\phi} \parallel p_{\theta}) + \alpha_T C_T(q_{\phi}(z) \parallel p_{\theta}(z)).$$

(14)

With the distribution consistency objective and the compositional inference model introduced in Sec. 3.4, we could train the latent variable generative model in a weakly/semi-supervised manner in terms of (i) incomplete data where $X$ is partially observed (e.g. missing attributes in feature vectors, or missing a modality in multi-modal dataset), and (ii) partial known dependency structure in $M^g$ and $M^p$.

Structure learning In this work, we show that our proposed framework is capable of learning the structure of Bayesian network $G^g$ and $G^p$ based on many existing structure learning methods efficiently, with gradient-based optimization techniques, which avoids searching over the discrete super-exponential space. Specifically, we show that our proposed framework can (i) represent the assumptions made about the structure of the true data distribution in the form of a set of structural regularization in the form of Bayesian networks $\{\mathcal{G}^k\}$ as the explicit inductive bias. A score-based structure learning objective is then introduced where $\mathcal{L}_{\text{str\_reg}}$ plays a vital role in scoring each candidate structure; and (ii) utilize the non-stationary data from multiple environments (Hyvärinen et al., 2019; Arjovsky et al., 2019; Ke et al., 2019) as additional observed random variables. We show the score-based structure learning objective as below

$$\min_{m^g, m^p} \mathcal{L}_{\text{score}} = \mathcal{L}_{\text{dist}} + \mathcal{L}_{\text{str\_reg}} + \mathcal{L}_{\text{sparsity}}.$$ 

(15)

We assume a jointly factorized Bernoulli distribution prior for structure variable $M^g$ and $M^p$, parametrized by $\rho^q$ and $\rho^p$. We use the gumbel-softmax trick proposed by (Jang et al., 2017; Maddison et al., 2017; Balog et al., 2017) as gradient estimators. Following the Bayesian Structural EM (Friedman, 1998; Elidan & Friedman, 2005) algorithm, we optimize the model alternatively between optimizing distributions $\mathcal{L}(q_{\phi}, p_{\theta})$ and structure variables $\mathcal{L}_{\text{score}}(m^g, m^p)$. We present the full algorithm to train the proposed generative model with optional structure learning procedure in Alg. 1.
Table 2. A unified view of {single/multi}-(modal/domain/view) models. \( C_i \) is referred to as the definition in Table 1. \( G \) is referred to as the Bayesian networks in Figure 1, 2. We use \( N \) to denote the number of views/domains/modals. We use ① to denote shared/private latent space decomposition, and use ② to denote dependency structure learning. Please see Appendix. A.1 for the full table.

| MODELS     | N | ① | ② | \( G^q \)                  | \( G^p \)                  | \( L_{dist} \) | \( L_{str\_reg} \) |
|------------|---|----|----|------------------------|------------------------|----------------|------------------|
| VAE        | 1 | ×  | ×  | \([\mathcal{G}^q_{single}]\) | \([\mathcal{G}^p_{single}]\) | [1, \( C_1 \)] | []               |
| GAN        | 1 | ×  | ×  | \([\mathcal{G}^p_{single}]\) | [1, \( C_2 \)] | [1, \( G^\text{InfoGAN} \)] | []               |
| INFOGAN    | 1 | ×  | ×  | \([\mathcal{G}^p_{single}]\) | [1, \( C_2 \)] | [1, \( G^\text{InfoGAN} \)] | []               |
| \( \beta \)-VAE | 1 | ×  | ×  | \([\mathcal{G}^q_{single}]\) | \([\mathcal{G}^p_{single}]\) | [1, \( C_1 \)], [\( \beta - 1, C_3 \)] | \([\beta - 1, G^\beta] \) |
| \( \beta \)-TCVAE | 1 | ×  | ×  | \([\mathcal{G}^q_{single}]\) | \([\mathcal{G}^p_{single}]\) | [1, \( C_1 \)], [\( \alpha_2, C_2 \)] | \([\beta, G^\beta] \) |
| JMVAE      | 2 | ×  | ×  | \([\mathcal{G}^q_{joint}]\) | \([\mathcal{G}^p_{joint}]\) | [1, \( C_1 \)] | [\( \beta_1, G^\text{str\_cross}(x_i) \)] |
| MVAE       | \( N \) | ×  | ×  | \([\mathcal{G}^q_{joint}, \mathcal{G}^q_{marginal}]\) | \([\mathcal{G}^p_{joint}]\) | [1, \( C_1 \)] | [\( \beta_1, G^\text{str\_marginal}(x_i) \)] |
| Wyner      | 2 | ✓  | ×  | \([\mathcal{G}^q_{joint}, \mathcal{G}^q_{marginal}]\) | \([\mathcal{G}^p_{joint}]\) | [1, \( C_1 \)] | [\( \beta_1, G^\text{str\_cross}(x_i), [\beta_1, G^\text{str\_private}(x_i)] \)] |
| OURS-MM    | \( N \) | ✓  | ✓  | \([\mathcal{G}^q_{full}]\) | \([\mathcal{G}^p_{full}]\) | [1, \( C_0 \)] | [\( \beta_1, G^\text{str\_cross}(\{x_i\}) \)] |

4. Case study: Generative Data Modeling

In this section, we show various types of generative data modeling can be viewed as a structured latent space learning problem, which can be addressed by our proposed framework in a principled way.

[Figure 1. Bayesian networks for single-modal models]

4.1. Single-modal generative model

Framework specification In single-modal data generative modeling setting, we have \( N = 1 \) observed variable \( X \equiv [X_1] \) which could be in image, text or other modalities, and we only incorporate private latent variables \( U \). We abuse the notation a little by assuming \( M \) latent variables \( U \equiv [U_1, U_2, \ldots, U_M] \).

A unified view We show that our proposed model unifies many existing generative models. We show that we can impose disentanglement as a special case of the structural regularization in latent space to obtain different existing disentangled representation learning methods. We summarize how existing generative models can be unified within our proposed information-theoretic framework in Table 2. As an interesting example, we show that we can derive the \( \beta \)-vae objective with \( L = C_1 + (\beta - 1)C_3 + (\beta - 1)L_{str\_reg}(G^\beta) \), where we impose the structural regularization \( (\beta - 1)D(q_{\theta} || G^\beta) \). In this way, we also established connections to the results in (Hoffman et al., 2017; Mathieu et al., 2019) that \( \beta \)-vae is optimizing ELBO with a \( q_{\phi} \)-dependent implicit prior \( r(u) \propto q_{\phi}(u)^{1-\beta}p_{\theta}(u)\beta \), we achieve this in a symmetric way by using a \( p_{\theta} \)-dependent posterior \( q_{\phi}(z | x) \propto p_{\theta}(z) \prod_{i=1}^N \frac{q_{\phi}(e_i | x_i)}{p_{\theta}(e_i | x_i)} \). We further show that how we can unify other total-correlation based disentangled representation learning models (Chen et al., 2018; Esmaeili et al., 2019; Kim & Mnih, 2018) by explicitly imposing Bayesian structure \( G^p \) as structural regularization. We include detailed discussions and proofs in Appendix. A.2.

4.2. Multi-modal/domain/view generative model

Problem setup We represent the observed variables as \( X_{1:N} \equiv [X_1, X_2, \ldots, X_N] \), where we have \( N \) observed variables in different domains\(^3\) and they might be statistically dependent. We thus aim to learn latent factors \( Z \) that explains the potential correlations among \( X \). Meanwhile, we also learn latent factors \( U_1 \) that explains the variations exclusive to one specific observed variable \( X_i \). In this way, we could achieve explicit control over the domain-dependent and domain-invariant latent factors. For more details of the data generation process for this task and the model, please see Appendix. B.1.

\(^3\)We use the word domain to represent domain/modality/view.
Figure 2. Bayesian networks of various inference, generation models and structural regularizations in multi-modal/domain/view setting.

**A unified view** We summarize the key results of unifying many existing multi-domain generative models in Table 2. We prove and discuss some interesting connections to related works in more details in Appendix A.3, including BiVCCA (Wang et al., 2016), JMVAE (Suzuki et al., 2017), TELBO (Vedantam et al., 2018), MVAE (Wu & Goodman, 2018), WynerVAE (Ryu et al., 2020), DIVA (Ilse et al., 2019) and CorEx (Steeg & Galstyan, 2014a;b; 2016; Gao et al., 2019).

**Framework specification** We present a specific implementation of our proposed framework for multi-domain generative modeling here. We show that it generalizes some heuristics used in previous models and demonstrates its effectiveness in several standard multi-modal datasets. We use \( \mathcal{L}_{\text{dist}} \) in Table 1 to learn consistent inference model and joint, marginal, conditional generation model over \( (X, Z, U) \). To embed multi-domain data into a shared latent space, we use the structural regularization that enforces Markov conditional independence structure \( X^S \rightarrow Z \rightarrow X^G \). This structural regularization can be represented by \( G^S_{\text{str}} \) in Figure 2, where \( X \equiv [X^S, X^G] \) is a random bi-partition of \( X \). Then we show that the objective can be upper-bounded by \( \mathcal{L} = \mathcal{L}_{\text{dist}} + \mathcal{L}_{\text{str-reg}} \leq \mathcal{L}_x + \mathcal{L}_u + \mathcal{L}_z \), where \( \mathcal{L}_x = -E_{q_\phi(x, u | z)} \log p_\theta(x \mid z, u) \), \( \mathcal{L}_u = E_{q_\phi(x)} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u)) \) and \( \mathcal{L}_z = \sum_{i=0}^N E_{q_\phi(z_i)} D_{KL}(q_\phi(z \mid x_i) \parallel q_\phi(z \mid x_i)) \). We use \( q_\phi(z \mid x_0) \equiv E_{q_\phi(z \mid x_0)} \) for the simplicity of notations. We further show that for each latent variable \( Z_j \), \( \mathcal{L}_z \), term can be viewed as a generalized JS-divergence (Nielsen, 2019) among \( q_\phi(z_j \mid x_i) \) for \( i \in \{1, \ldots, N\} \) using geometric-mean weighted by \( m^j \), which can be seen as a generalization of the implicit prior used in \( \beta\text{-vae} \) as discussed in 4.1. The detailed proof is presented in Appendix A.3.

\[
\mathcal{L}_{z_j} = D_{JS}^m(q_\phi(z_j \mid x_0), q_\phi(z_j \mid x_1), \ldots, q_\phi(z_j \mid x_N))
\]

(16)

Figure 3. Cross-domain generation samples. The leftmost column shows conditioned inputs.

**Experiment** We validate the effectiveness of proposed model in multi-view/modal data modeling setting on bi-modal MNIST-Label, MNIST-SVHN and bi-view MNIST-MNIST-Plus-I dataset. We show the generated samples in Figure 3. The left panel in the figure contains the examples of MNIST-style samples generated by the model trained on MNIST-SVHN dataset when conditioned on SVHN data examples. We can observe that the model is using the shared latent variable \( Z \) and private latent variables \( U \) to successfully generate the MNIST-style samples of same digit as the SVHN inputs. On the other hand, the right panel contains the examples of MNIST-style sample generated by the model trained on MNIST-Plus-I dataset by conditioning on MNIST example. We can observe that the model is successfully generating \( m + 1 \) digit images when conditioned on \( m \) digit input. More detailed results are included in the Appendix B.1.

**5. Case study: Fair Representation Learning**

In this section, we show that fair representation learning can be viewed as a structured latent space learning problem, where we aim to learn a latent subspace that is invariant to sensitive attributes while informative about target label.

**Problem setup** We use \( [X, A, Y] \) to represent the observed variables, where the variable \( X \) represents the multivariate raw observation like pixels of image sample, the variable \( A \) represents the sensitive attributes, and the variable \( Y \) represents the target label to be predicted. Following the
Table 3. Fair representation learning results on German and Adult datasets.

| Model         | Adult ACC | DEO | German ACC | DEO |
|---------------|-----------|-----|------------|-----|
| Naive SVM     | 0.80      | 0.09| 0.74 ± 0.05| 0.12 ± 0.05|
| SVM           | 0.79      | 0.08| 0.74 ± 0.03| 0.10 ± 0.06|
| NN            | 0.84      | 0.14| 0.74 ± 0.04| 0.47 ± 0.19|
| NN + χ²       | 0.83      | 0.03| 0.73 ± 0.03| 0.25 ± 0.14|
| FERM          | 0.77      | 0.01| 0.73 ± 0.04| 0.05 ± 0.03|
| Ours-MMD      | 0.83      | 0.02| 0.72 ± 0.07| 0.07 ± 0.09|
| Ours-TC       | 0.81      | 0.02| 0.74 ± 0.08| 0.08 ± 0.14|
| Ours-MINE     | 0.79      | 0.01| 0.70 ± 0.11| 0.05 ± 0.11|

The same setting in previous works (Song et al., 2019; Creager et al., 2019), the target label is not available during training phase. A linear classifier using learned representation is trained to predict the held-out label Y in testing time. We focus on the Difference of Equal Opportunity (DEO) notion in this work (Hardt et al., 2016). For the details of the data generation process, please see Appendix. A.4.

Framework specification

We learn a joint distribution over [X, A, Z, U] with the framework proposed. The shared latent variable Z aims to explain the hidden correlation among X and Z. We also enforce two structural regularizations, represented by two Bayesian networks $G_{\text{inv}}^{str}$ and $G_{\text{str}}^{\text{informative}}$. The aim of $G_{\text{inv}}^{\text{informative}}$ is to learn the private latent variables $U_X$ as the hidden factors that are invariant to the change of Z. Meanwhile, the aim of $G_{\text{str}}^{\text{informative}}$ is to preserve as much information about X in Z. $M^s$ and $M^p$ are illustrated by $G^q$ and $G^p$ in Figure 4 correspondingly. Then we have $p_\theta(x)q(z | x) = p_\theta(x,a)q(z | x, a) = L_q$ (17) and $p_{\theta}^{const}(z | x) = L_q$ (17) corresponding environment index. The goal of this task is predict Y from X in a way that the performance of the predictor in the presence of the worst E is optimal. We derive an information-theoretic objective for out-of-distribution generalization task on Colored-MNIST dataset introduced in (Arjovsky et al., 2019). For more details of this experiment, please see the Appendix. B.3 as well as the original work (Peters et al., 2015; Arjovsky et al., 2019).

Framework specification

As our structural regularization, we use the Bayesian network $G_{\text{ood}}^{\text{str}}$ in Figure 5. The purpose of $G_{\text{ood}}^{\text{str}}$ is to enforce that Z is sufficient statistic in making the prediction of Y and that $E \perp Y | Z$. We present the derived learning objective here

$$L_{\text{info}} = L_{\text{dist}} + \beta_1 D_{\text{KL}}(q_{\phi}(z | x, e, y) || q_{\phi}(z | x)) + \beta_2 I_q(x, e, y | z)$$

We further show that the idea in (Arjovsky et al., 2019) can be directly integrated into our proposed framework by imposing stable $M^p$ structure as constraints across environments, measured by gradient-penalty, as discussed in Appendix. A.5.

Experiments

We validate the proposed model on the Colored-MNIST classification task introduced in (Arjovsky et al., 2019). We also take the advantage of our proposed framework as a generative model that we could perform semi-supervised learning, where we use only 50% labeled data. We include more training setting details in Appendix. B.3. We compare our model against the baselines in

Figure 5. Bayesian networks for out-of-distribution generalization task. E in the diagram represents the index of the environmental factor, not the real value of E in the data generation process.
Table 4. Out-of-distribution generalization results on Colored-MNIST

| Model     | ACC. TRAIN ENVs. | ACC. TEST ENV. |
|-----------|------------------|----------------|
| RANDOM    | 50               | 50             |
| OPTIMAL   | 75               | 75             |
| ORACLE    | 73.5 ± 0.2       | 73.0 ± 0.4     |
| ERM       | 87.4 ± 0.2       | 17.1 ± 0.6     |
| IRM       | 70.8 ± 0.9       | 66.9 ± 2.5     |
| OURS-FULL | 67.8 ± 6.8       | 62.1 ± 6.1     |
| OURS-SEMI | 71.4 ± 6.1       | 58.7 ± 7.2     |

Table 4. We see that our proposed information-theoretic objective achieves comparable performance in both supervised and semi-supervised setting on the test-environment.

7. Conclusion

In this work, we propose a general information-theoretic framework for learning structured latent factors from multivariate data, by generalizing the multivariate information bottleneck theory. We show that the proposed framework can provide an unified view of many existing methods and insights on new models for many different challenging tasks like fair representation learning and out-of-distribution generalization.

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A. Proofs

A.1. Proofs of results in section 3 framework

A.1.1. Generalized MIB objective

We generalized the original MIB structural variational learning objective in equation 8. We show that by choosing $C_1 = D_{KL}(q \parallel p \theta)$, $T = 1$ and $G^1 = G^0$, $K = 1$, we can recover the original MIB objective equation 5.

**Proposition 1.** Let $X \sim P(X)$, and let $G^0$ be an empty Bayesian network over $X$. Then

$$\mathbb{D}(p \parallel G^0) = \min_{q \bowtie G^0} D_{KL}(p \parallel q) = I_p(X) - I_{p^G}(X) = I_p(X)$$  \hspace{1cm} (19)

**Proof.** By definition, we have $I_{p^G}(X) = 0$. \hfill \Box

Then we can see that our objective is equivalent to the original MIB objective equation 5 when $\alpha_1 = 1, \beta_1 = \gamma$.

$$L = L_{dist} + L_{str\_reg} = \alpha_1 D_{KL}(q \parallel p \theta) + \beta_1 \mathbb{D}(q \parallel G^0) = \alpha_1 D_{KL}(q \parallel p \theta) + \beta_1 I_{q^G}$$  \hspace{1cm} (20)

A.1.2. Derivation of equation 12

$$q_\phi(z \mid x^S) \propto p_\theta(z) \prod_{i \in S} \frac{q_\phi(z \mid x_i)}{p_\theta(z)}$$

$$= p_\theta(z) \prod_{i \in S} \prod_{j=1}^M (\tilde{q}_\phi(z_j \mid x_i))^{m_{ij}}$$

$$= \prod_{j=1}^M \left( p_\theta(z_j) \prod_{i \in S} (\tilde{q}_\phi(z_j \mid x_i))^{m_{ij}} \right)$$  \hspace{1cm} (21)

A.1.3. Full table 2

We show the full Table 2 in Table 5.

A.2. Proof of results in section 4.1 single-modal generative mode

A.2.1. Unifying disentangled generative models

**$\beta$-VAE** For $\beta$-vae we have

$$L = L_{dist} + L_{str\_reg}$$

$$= C_1 + (\beta - 1)C_3 + (\beta - 1)L_{str\_reg}(G^0)$$

$$= C_1 + (\beta - 1)C_3 + (\beta - 1)\mathbb{D}(q \parallel G^0)$$

$$= \mathbb{E}_{q_\phi} \log p_\theta(x \mid u) + \mathbb{E}_{q_\phi} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u)) + (\beta - 1)D_{KL}(q_\phi(u) \parallel p_\theta(u)) + (\beta - 1)I_q(x ; u)$$

$$= \mathbb{E}_{q_\phi} \log p_\theta(x \mid u) + (1 + \beta - 1)D_{KL}(q_\phi(u) \parallel p_\theta(u)) + (1 + \beta - 1)I_q(x ; u)$$

$$= \mathbb{E}_{q_\phi} \log p_\theta(x \mid u) + \beta \mathbb{E}_{q_\phi} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u))$$

$$\equiv L_{\beta\_vae}$$

where we include the structural regularization $L_{str\_reg}$ using an empty Bayesian network $G^{\beta\_vae} = G^0$. Thus we show that the $\beta$-vae objective is equivalent to imposing another empty Bayesian network structure in the latent space which implies the independent latent factors.

**TCVAE (Chen et al., 2018)** We further show that how we can unify other total-correlation based disentangled representation learning models (Chen et al., 2018; Esmaeili et al., 2019; Kim & Mnih, 2018) by explicitly imposing Bayesian structure $G^P$
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Table 5. A unified view of \{single/multi\}-\{modal/domain/view\} models

| MODELS       | N     | \( \mathcal{G}^q \) | \( \mathcal{G}^p \) | \( \mathcal{L}_{\text{dist}} \) | \( \mathcal{L}_{\text{str_reg}} \) |
|--------------|-------|----------------------|----------------------|----------------------------------|-----------------------------------|
| VAE          | 1     | \( \mathcal{G}_{\text{single}}^q \) | \( \mathcal{G}_{\text{single}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{single}}^p] \) |
| ICA          | 1     | \( \mathcal{G}_{\text{single}}^q \) | []                   | []                               | \( [\beta - 1, C_3] \) |
| GAN          | 1     | \( \mathcal{G}_{\text{single}}^q \) | \( \mathcal{G}_{\text{single}}^p \) | \( [1, C_2] \) | [] |
| INFOGAN      | 1     | \( \mathcal{G}_{\text{single}}^q \) | []                   | []                               | \( [1, \mathcal{G}_{\text{InfoGAN}}^p] \) |
| \( \beta \)-VAE | 1     | \( \mathcal{G}_{\text{single}}^q \) | \( \mathcal{G}_{\text{single}}^p \) | \( [1, C_1], [\beta - 1, C_3] \) | \( [\beta - 1, \mathcal{G}^p] \) |
| \( \beta \)-TCVAE | 1     | \( \mathcal{G}_{\text{single}}^q \) | \( \mathcal{G}_{\text{single}}^p \) | \( [1, C_1], [\alpha_2, C_3] \) | \( [\beta, \mathcal{G}^p] \) |
| BiVCCA       | 2     | \( \mathcal{G}_{\text{marginal}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [\alpha_1, C_4(x, z)] \) | [] |
| JMVAE        | 2     | \( \mathcal{G}_{\text{joint}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{cross}}^p(x)] \) |
| TELBO        | 2     | \( \mathcal{G}_{\text{joint}, \text{marginal}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{marginal}}^p(x)] \) |
| MVAE         | \( \times \) | \( \mathcal{G}_{\text{joint, marginal}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{cross}}^p(x)] \) |
| WYNER        | 2     | \( \mathcal{G}_{\text{joint, marginal}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{cross}}^p(x)], [\beta, \mathcal{G}_{\text{private}}^p(x)] \) |
| DIVA         | 3     | \( \mathcal{G}_{\text{marginal}}^q \) | \( \mathcal{G}_{\text{joint}}^p \) | \( [1, C_1] \) | \( [\beta, \mathcal{G}_{\text{cross}}^p(x)] \) |
| OURS-MM      | \( \times \) | \( \mathcal{G}_{\text{full}}^q \) | \( \mathcal{G}_{\text{full}}^p \) | \( [1, C_0] \) | \( [\beta, \mathcal{G}_{\text{cross}}(x)] \) |

as structural regularization, where a factorized prior distribution is assumed.

\[
\mathcal{L} = C_1 + \alpha_2 C_3 + \beta \mathcal{L}_{\text{str_reg}}
\]

\[
\mathcal{L}_{\text{str_reg}} = \mathbb{D}(q_{\phi} \parallel \mathcal{G}^p) = \mathcal{L}_q^0 - \mathcal{L}_q^p = \sum_j M \mathcal{I}_q(x; u_j) - \mathcal{I}_q(u) = \mathcal{I}_q(u) - \mathcal{I}_q(u \mid x) = \mathcal{I}_q(u) \equiv TC(u)
\]  

(23)

Since we assume a factorized posterior distribution \( q_{\phi}(u \mid x) \), we have \( \mathcal{I}_q(u \mid x) = 0 \) in the last line of above objective. Thus the total-correlation minimization term emerges as a structural regularization term naturally in our framework.

A.3. Proof of results in section 4.2 multi-modal/domain/view generative model

A.3.1. Unifying multi-modal/domain/view generative models

We show that we can obtain several representative multi-modal generative models as special cases of our proposed framework here.

**JMVAE (Suzuki et al., 2017)** We can see that the objective of JMVAE is a special case of our proposed objective when \( N = 2 \).

**Wyner-VAE (Ryu et al., 2020)** By using structural regularization \( \mathbb{D}(q_{\phi} \parallel \mathcal{G}_{\text{cross}}^p(x_i)) \), we show that we can obtain the mutual information regularization term appeared in the learning objective of Wyner-VAE (Ryu et al., 2020)

\[
\mathcal{L}_{\text{str_reg}} = \mathbb{D}(q_{\phi} \parallel \mathcal{G}_{\text{cross}}^p(x_i)) = \mathcal{I}_q^0 - \mathcal{I}_q^p
\]

\[
= \mathcal{I}_q(x_1; u_1) + \mathcal{I}_q(x_2; u_2) + \mathcal{I}_q(x_1, x_2; z) - \mathcal{I}_q(x_1; u_1) - \mathcal{I}_q(x_2; u_2) = \mathcal{I}_q(x_1, x_2; z)
\]

(24)

**CorEx (Steeg & Galstyan, 2014a)** One of the most interesting model with similar goal to decorrelate observed variables is
CorEx (Steeg & Galstyan, 2014a;b; 2016; Gao et al., 2019), whose objective is

\[
\max_{G_j, q \phi \mid x \mid G_j} \mathcal{L}_{\text{CorEx}} = \sum_{j=1}^{M} TC(x_{G_j}) - TC(x_{G_j} \mid z_j)
\]  

(25)

For each \(1 \leq j \leq M\), CorEx objective aims to search for a latent variable \(Z_j\) to achieve maximum total-correlation reduction \(TC(x_{G_j}) - TC(x_{G_j} \mid z_j)\) of a group of observed variables \(X_{G_j}\). We use \(M^{q}_{i,j}\) and \(M^{p}_{i}z\) to represent \(G_j\) equivalently, then our objective is

\[
\mathcal{L}_{\text{dist}} = \mathbb{D}(q_{\phi} \parallel G^p) = \mathcal{I}_q^{\phi} - \sum_{i=1}^{N} \mathcal{I}_q(z_j \mid x_i) = \sum_{j=1}^{M} \sum_{i=1}^{N} m^q_{i,j} \mathcal{I}_q(z_j \mid x_i) + \sum_{j=1}^{M} \left[ \mathcal{I}_q(x^{m^q_j} \mid z_j) - \sum_{i=1}^{N} \sum_{j=1}^{M} m^q_{i,j} \mathcal{I}_q(z_j \mid x_i) - \sum_{i=1}^{N} \mathcal{I}_q(z^{m^q_j} \mid x_i) \right] \leq \sum_{j=1}^{M} \mathcal{I}_q(x^{m^q_j} \mid z_j) - \sum_{i=1}^{N} \mathcal{I}_q(z^{m^q_j}) + \sum_{i=1}^{N} \mathcal{I}_q(z^{m^q_j}) \]

\(= -\mathcal{L}_{\text{CorEx}} + \sum_{i=1}^{N} \mathcal{I}_q(z^{m^q_j})\)

(26)

Thus with structural regularization \(G^p\) we obtained an objective coincides with CorEx-based variational autoencoder (Gao et al., 2019), which is also upper-bound of original CorEx objective (Steeg & Galstyan, 2014a) with additional disentangle-ment regularization over latent variables.

A.3.2. DERIVATION OF OBJECTIVE EQUATION 16

We show the detailed derivation of the learning objective of our multi-domain generative model here. As introduced in 4.2, we impose \(N\) structural regularization for each individual \(X^i = \{X_i\}\) as \(\mathbb{D}(q_{\phi} \parallel G^\text{str}_{\text{cross}}(\{X_i\}))\). First we hvae

**Proposition 2.** We have following upper-bound

\[
\frac{1}{N} \sum_{i=1}^{N} \mathbb{D}(q_{\phi} \parallel G^\text{str}_{\text{cross}}(\{X_i\})) \leq \mathcal{L}_u + \sum_{i=1}^{N} \mathbb{E}_{q_{\phi}} \mathcal{D}_{KL}(q_{\phi}(z \mid x) \parallel q_{\phi}(z \mid x_i))
\]

(27)
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Proof.

\[
\frac{1}{N} \sum_{i=1}^{N} D(q_\phi \parallel G_{\text{cross}}^\text{str}(\{x_i\})) = I_q(u : x) + \frac{1}{N} \sum_{i=1}^{N} \left[ I_q(z ; x) - I_q(z ; x_i) - \sum_{k \neq i} I_q(z ; x_k) \right]
\]

\[
= I_q(u : x) + \frac{1}{N} \sum_{i=1}^{N} I_q(z ; x) + \frac{1}{N} \sum_{i=1}^{N} \left[ -I_q(z ; x_i) + \sum_{k \neq i} I_q(z ; x_k) \right]
\]

\[
= I_q(u : x) + I_q(z ; x) - \sum_{i=1}^{N} I_q(z ; x_i)
\]

\[
= \mathbb{E}_{q_\phi} D_{KL}(q_\phi(u \mid x) \parallel q_\phi^{mg}(u)) + \sum_{i=1}^{N} \mathbb{E}_{q_\phi} D_{KL}(q_\phi(z \mid x) \parallel q_\phi^{mg}(z \mid x_i))
\]

\[
= \mathbb{E}_{q_\phi} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u)) + \sum_{i=1}^{N} \mathbb{E}_{q_\phi} D_{KL}(q_\phi(z \mid x) \parallel q_\phi(z \mid x_i))
\]

\[
- \mathbb{E}_{q_\phi} D_{KL}(q_\phi^{mg}(u) \parallel p_\theta(u)) - \sum_{i=1}^{N} \mathbb{E}_{q_\phi} D_{KL}(q_\phi^{mg}(z \mid x) \parallel q_\phi(z \mid x_i))
\]

\[
\leq \mathbb{E}_{q_\phi} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u)) + \sum_{i=1}^{N} \mathbb{E}_{q_\phi} D_{KL}(q_\phi(z \mid x) \parallel q_\phi(z \mid x_i))
\]

\[
= \mathcal{L}_u + \sum_{i=1}^{N} \mathbb{E}_{q_\phi} D_{KL}(q_\phi(z \mid x) \parallel q_\phi(z \mid x_i))
\]

\[\square\]

where \(q_\phi^{mg}(u) = \mathbb{E}_{q_\phi} q_\phi(u \mid x)\) and \(q_\phi^{mg}(z \mid x_i) = \mathbb{E}_{q_\phi(z \mid x_i)} q_\phi(z \mid x)\) denote the induced marginalization of \(q_\phi(x, u, z)\). Note that by using the above upper-bound, the inference network distribution \(q_\phi(z \mid x_i)\) introduced in 3.4 is trained to approximate the true marginalization \(q_\phi^{mg}(z \mid x)\). Thus we have following full objective

\[
\mathcal{L} = \mathcal{L}_\text{dist} + \mathcal{L}_\text{str-reg} = D_{KL}(q_\phi(x, z, u) \parallel p_\theta(x, z, u)) + \frac{1}{N} \sum_{i=1}^{N} D(q_\phi \parallel G_{\text{cross}}^\text{str}(\{x_i\}))
\]

\[
= -\mathbb{E}_{q_\phi(x, u \mid x)} \log p_\theta(x \mid z, u)
\]

\[
+ \mathbb{E}_{q_\phi(x)} D_{KL}(q_\phi(u \mid x) \parallel p_\theta(u))
\]

\[
+ \sum_{i=0}^{N} \mathbb{E}_{q_\phi(x)} D_{KL}(q_\phi(z \mid x) \parallel q_\phi(z \mid x_i))
\]

\[
\equiv \mathcal{L}_x + \mathcal{L}_u + \mathcal{L}_z
\]

We use \(q_\phi(z \mid x_i) = p_\theta(z)\) for the simplicity of notations. We further show that \(\mathcal{L}_z\) can be viewed as a generalized JS-divergence for the reverse KL-Divergence \((\text{Nielsen}, 2019)\). We decompose \(\mathcal{L}_z\) regarding each latent variable \(Z_j\),

\[
\mathcal{L}_z = \sum_{j=1}^{M} \mathcal{L}_{z_j}, \quad q_\phi(z_j \mid x) \propto \prod_{i=0}^{N} q_\phi(z_j \mid x_i)^{\gamma_{ij}}
\]

\[
\mathcal{L}_{z_j} = D_{\text{JS}}^\ast(q_\phi(z_j \mid x_0), q_\phi(z_j \mid x_1), \ldots, q_\phi(z_j \mid x_N))
\]

\[
\sum_{i=0}^{N} \gamma_i = 1, \quad \gamma_{0j} = 1 - \sum_{i=1}^{N} m_{ij}^0, \quad \gamma_{ij} = m_{ij}^0, \quad i > 0
\]

where we use \(\text{KL}^\ast\) to denote the reverse KLD and following the same notation in \((\text{Nielsen}, 2019)\) for the generalized JSD.
A.4. Proof of results in section 5 case study: fair representation learning

We show the detailed derivation of the learning objective 17 here.

\[
L = L_{\text{dist}} + L_{\text{str-reg}} = D_{KL}(q_\phi(x, z, u) \parallel p_\theta(x, z, u)) + \beta_1 D(q_\phi \parallel G_{\text{informative}}) + \beta_2 D(q_\phi \parallel G_{\text{invariant}}) \\
= D_{KL}(q_\phi \parallel p_\theta) + \beta_1 I_q(x; a | z) + \beta_2 I_q(z; u) + \text{const} \\
\leq -\mathbb{E}_{q_\phi} \log p_\theta(x, a | z, u) + (1 + \beta_1) D_{KL}(q_\phi(z | x, a) \parallel p_\theta(z)) + \text{const}
\]  

(30)

We can interpret this derived learning objective as first seeking for a succinct latent representation \( Z \) that captures the sufficient correlation between \( X \) and \( A \), then \( Z \) is served as a proxy variable to learn an informative representation \( U \) with all information relevant to \( A \) eliminated by minimizing \( I_q(z; u) \).

A.5. Details of section 6 case study: invariant risk minimization

We show that the idea in (Arjovsky et al., 2019) can be directly integrated into our proposed framework by imposing stable \( M^p \) structure as constraints across environments, measured by gradient-penalty term shown below

\[
L_{\text{gp}} = L_{\text{dist}} + \mathbb{E}_{q_\phi(e)} \| \nabla_{M^p} \mathcal{L}_{\text{score}} \|
\]

(31)

B. Experiments

B.1. Generative modeling

Datasets Following the same evaluation protocol proposed by previous works (Ryu et al., 2020; Wu & Goodman, 2018), we construct the bi-modal datasets MNIST-Label by using the digit label as a second modality, MNIST-SVHN by pairing each image sample in MNIST with another random SVHN image sharing the same digit label and a bi-view dataset MNIST-MNIST-Plus-1 by pairing each MNIST sample \( X_1 \) with another random sample \( X_2 \) correlated as \( \text{label}(X_1) + 1 = \text{label}(X_2) \).

We illustrate the data generating process using Bayesian networks in Figure 6.

![Bayesian networks for illustrating the data generating process of MNIST-SVHN dataset and MNIST-PLUS-1 dataset.](image)

Figure 6. Bayesian networks for illustrating the data generating process of MNIST-SVHN dataset and MNIST-PLUS-1 dataset.

Training details and hyper-parameters For MNIST-Label dataset, we use MLPs with 2 hidden layers for both encoders and decoders, following the same neural network architecture in (Wu & Goodman, 2018). The dimension of \( Z \) modeling the shared information is 2. The dimension of \( U_1 \) modeling MNIST image is 20. We don’t include \( U_2 \) in this setting and set the dimension of \( U_2 \) to 0. For MNIST-SVHN dataset, the dimension of \( Z \) is 2, the dimension of \( U_1 \) for MNIST is 20 and the dimension of \( U_2 \) for SVHN is 20. For MNIST-MNIST-Plus-1 dataset, the dimension of \( Z \) is 2, and the dimension of \( U_1 \) for MNIST is 20. We train the model using the Adam optimizer with a learning rate starting from 0.001, and decay the learning rate by a factor 0.1 whenever a validation loss plateau is found during training. We train the model up to 1000 epochs for all datasets. We learn the structural variable \( M \) with \( \text{steps_dist} = 1 \) and \( \text{steps_str} = 3 \) in all experiments. We use the same neural network architectures for encoder and decoder as (Ryu et al., 2020) in MNIST-SVHN and MNIST-MNIST-Plus-1 datasets.

Qualitative results of MNIST-Label Due to the space limit constraint, we include the qualitative results of MNIST-Label experiment here. We show the conditionally generated samples in figure 7.
B.2. Fairness

Training details and hyperparameter sensitivity
We follow the same neural network architecture design and evaluation process in (Song et al., 2019). The dimension of $U$ is 10 for German and Adult datasets, the dimension of $Z$ is 5. We find that the experimental result is not sensitive to the dimension of $Z$ when it’s in range $2$ to $10$. We train the model up to 10000 epochs using Adam optimizer with learning rate 0.001, and decay the learning rate by a factor 0.1 when loss plateau is detected. We don’t train the structural variables in this experiment. We re-scale the likelihood in objective to make the loss terms balance for the consideration of training stability. Numbers in table 3 are evaluated with 10 random runs with different random seeds.

B.3. Out-of-Distribution Generalization

Colored MNIST
Colored MNIST is an experiment that was used in (Arjovsky et al., 2019), in which the goal is to predict the label of a given digit in the presence of varying exterior factor $e$. The dataset for this experiment is derived from MNIST. Each member of the Colored MNIST dataset is constructed from an image-label pair $(x, y)$ in MNIST, as follows.

1. Generate a binary label $\hat{y}_{obs}$ from $y$ with the following rule: $\hat{y}_{obs} = 0$ if $y \in \{0 \sim 4\}$ and $\hat{y}_{obs} = 1$ otherwise.
2. Produce $y_{obs}$ by flipping $\hat{y}_{obs}$ with a fixed probability $p$.
3. Let $x_{fig}$ be the binary image corresponding to $y$. 
4. Put $y_{obs} = \tilde{x}_{ch1}$, and construct $x_{ch1}$ from $\tilde{x}_{ch}$ by flipping $\tilde{x}_{ch1}$ with probability $p_e$.

5. Construct $x_{obs} = x_{fig} \times [x_{ch0}, (1 - x_{ch0}), 0]$. (that is, make the image red if $x_{ch1} = 1$ and green if $x_{ch1} = 0$.) Indeed, $x_{obs}$ has exactly same information as the pair $(x_{fig}, x_{ch1})$.

The goal of this experiment is to use the dataset with $p_e$ values in small compact range (training dataset) to train a model that can perform well on all ranges of $p_e$. In particular, we use the dataset with $p_e \in \{0.1, 0.2\}$ and evaluate the model on the dataset with $p_e = 0.9$. For more details of Colored MNIST experiment, please consult the original article.

Training details We follow the same neural network architecture design of encoder and evaluation process in (Arjovsky et al., 2019). The decoder is 1-layer MLP. We re-scale the likelihood terms to make the gradient norm of each one stays in the same magnitude. We train the model in a full-batch training manner, that the batch size is 50000. For semi-supervised training, we randomly partitioned the dataset into two halves and alternate between training $(X, E, Y)$ and $(X, E)$. The dimension of $Z$ is 4. Following the same practice in (Arjovsky et al., 2019), we use early-stopping on validation set as regularization. Numbers in table 4 are evaluated with 10 random runs with different random seeds. We illustrate the training dynamics of our model by plotting the accuracy progression in both training environments and testing environment in Figure 8.