Conditional Independence Testing via Latent Representation Learning

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Abstract—Detecting conditional independencies plays a key role in several statistical and machine learning tasks, especially in causal discovery algorithms, yet it remains a highly challenging problem due to dimensionality and complex relationships presented in data. In this study, we introduce LCIT (Latent representation based Conditional Independence Test)—a novel method for conditional independence testing based on representation learning. Our main contribution involves a hypothesis testing framework in which to test for the independence between $X$ and $Y$ given $Z$, we first learn to infer the latent representations of target variables $X$ and $Y$ that contain no information about the conditioning variable $Z$. The latent variables are then investigated for any significant remaining dependencies, which can be performed using a conventional correlation test. The empirical evaluations show that LCIT outperforms several state-of-the-art baselines consistently under different evaluation metrics, and is able to adapt really well to both non-linear and high-dimensional settings on a diverse collection of synthetic and real data sets.

Index Terms—conditional independence, hypothesis testing, representation learning, generative models, normalizing flows

I. INTRODUCTION

Conditional independence (CI) tests concern with the problem of testing if two random variables $X$ and $Y$ are statistically independent after removing all the influences coming from the conditioning variables $Z$ (denoted as $X \perp \!\!\!\!\!\perp Y \mid Z$), using the empirical samples from their joint distribution $p(X, Y, Z)$. More formally, we consider the hypothesis testing setting with:

- Null hypothesis $H_0 : X \perp \!\!\!\!\!\perp Y \mid Z$
- Alternative hypothesis $H_1 : X \not\perp \!\!\!\!\!\perp Y \mid Z$

With this functionality, CI tests have been extensively leveraged as the backbone of causal discovery algorithms which aim to disassemble the causal interrelationships embedded in the observed data. More specifically, in constraint-based causal discovery methods such as the PC algorithm and its variants [36], [37], CI tests are used to detect if each pair of variables has an intrinsic relationship that cannot be explained by any other intermediate variables, and so forth connectivity of those who do not share this kind of relation are progressively removed. The outputs from such methods are extremely valuable in many scientific sectors such as econometrics [15], neuroscience [4], machine learning [31], [32], [33], and especially bioinformatics [30], [42] where the behavioral links between genes, mutations, diseases, etc., are at the heart of curiosity.

Here we consider the continuous instance of the problem where $X, Y$, and $Z$ are real-valued random vectors or variables, which is significantly harder than the discrete case in general. This is because discrete probabilistic quantities are usually more tractable to be accurately estimated, in contrary with their continuous counterparts. In fact, many methods must resort to binning continuous variables into discrete values for their tests [39], [5], [41]. However, this technique is prone to loss of information and is erroneous in high dimensions due to the curse of dimensionality. This also highlights the inherent difficulty of CI testing in continuous domains.

From the technical perspective, CI tests can be roughly categorized into four major groups based on their conceptual essence, including distance-based methods, kernel-based methods, regression-based methods, and model-based methods. In distance-based methods [39], [8], [41], the direct characterization of CI, $p(x \mid z)p(y \mid z) = p(x, y \mid z)$ or $p(x \mid y, z) = p(x \mid z)$, is exploited and methods in this class aim to explicitly measure the difference between respective probability densities or distributions. These methods usually employ discretization, which has been discussed to be faulty as the data dimensionality increases.

Next, kernel-based methods [10], [46], [7], [38] adopt kernels to exploit high order properties of the distributions via sample-wise similarities in higher spaces. More concretely, variables are mapped into reproducing kernel Hilbert spaces (RKHS), where their conditional independence can be reflected by the partial uncorrelatedness of functions in the RKHS. However, as noted in [27], the performance of kernel-based methods may polynomially deteriorate w.r.t. the dimensionality of data as well.

The next group of CI tests is regression-based methods [12], [45], [44], [43], which transform the original CI testing problem into a more manageable problem of marginal independence testing between regression residuals. Typically, these methods suppose that $Z$ is a confounder set of $X$ and $Y$, meaning it causes both $X$ and $Y$ in the underlying generation process, and the generating functions are additive noise models (ANMs), so that the residuals can be fully retrieved without any remaining information from $Z$—by using suitable regression functions. While being simple, the application of regression-based methods is quite limited since in general there is a high chance that $Z$ is not a cause of $X$ or $Y$, or the generating mechanisms may have non-additive noises.

Finally, the last group of CI methods contain a diverse
Figure 1: The proposed Latent representation based Conditional Independence Test (LCIT) framework. First, $X$ and $Y$ are transformed into respective latent spaces using two Conditional Normalizing Flows (CNF) modules independently learned from samples of $(X, Z)$ and $(Y, Z)$, respectively. The latent variables ($\epsilon_X$ and $\epsilon_Y$), which have standard Gaussian distributions by design, are then used as inputs for a conventional correlation test. If $\epsilon_X$ and $\epsilon_Y$ are indeed uncorrelated then we accept the null hypothesis ($H_0: X \perp \!\!\!\perp Y | Z$), otherwise we reject the null hypothesis and accept the alternative ($H_1: X \not\!\!\!\perp \!\!\!\perp Y | Z$).

set of approaches leveraging learning algorithms as the main technical device. For example, in [29], [21], [18] the conditional mutual information (CMI) between $X$ and $Y$ given $Z$ is considered as the test statistics and estimated using $k$-nearest neighbors estimators. Additionally, methods utilizing generative adversarial neural networks (GAN) [3], [35] have also been proposed where new samples are generated to help simulate the null distributions of the test statistics. Also, in [34] the use of supervised classifiers is harnessed to differentiate between conditional independence and conditional dependence samples.

Present study. In this study, we offer a novel approach to test for conditional independence motivated by regression-based methods and executed via latent representation learning with normalizing flows. Our proposed method, called Latent representation based Conditional Independence Testing (LCIT)$^1$, learns to infer the latent representations of $X$ and $Y$ conditioned on $Z$, then tests for their unconditional independence.

To infer the latent variables, we make use of Normalizing Flows (NF) [40], [22], which is a subset of generative modeling methods designed to represent complex distributions using much simpler “base” distributions via the use of a sequence of bijective transformations. Here, the latent variables, i.e., the “bases” in the NF framework, are chosen to be Gaussians so that their independence can be tested with a correlation test where the $p$-value has a simple close-form expression, unlike many approaches in the literature of conditional independence testing that require bootstrapping since their test statistics have non-trivial null distributions [46], [29], [3], [21], [35], [44], [43].

We demonstrate the effectiveness of our method in conditional independence testing with extensive numerical simulations, as well as in real datasets. The empirical results show that LCIT outperforms existing state-of-the-art methods in a consistent manner.

Contributions. This paper offers three key contributions summarized as follows:

1) We present a conversation of conditional independence into unconditional independence of “latent” variables via invertible transformations of target variables, adjusted on the conditioning set. This characterization allows us to operate with the conventional marginal independence testing problem which is less challenging than the original conditional problem.

2) We introduce a new conditional independence testing algorithm, called Latent representation based Conditional Independence Testing (LCIT), which harnesses a Conditional Normalizing Flows framework to convert target variables into corresponding latent representations, where their uncorrelatedness entails conditional independence in the original space. To the best of our knowledge, this is the first time Normalizing Flows is applied into the problem of conditional independence testing. Additionally, deviating from many of the existing non-parametric tests, LCIT can estimate the $p$-value computationally cheaper than methods involving bootstrapping or permutation. See Figure 1 for an illustration of our framework.

3) We demonstrate the effectiveness of the proposed LCIT

$^1$Source code and related data are available at https://github.com/baosws/LCIT
method with a comparison against various state-of-the-art baselines on both synthetic and real datasets, where LCIT is showed to outperform other methods in several metrics.

**Paper organization.** In the following parts of the paper, we first briefly highlight major state-of-the-art ideas in the literature of conditional independence hypothesis testing in Section II. Then, in Section III we describe in detail our proposed LCIT method for conditional independence testing. Next, in Section IV we perform experiments to demonstrate the strength of LCIT in both synthetic and real data settings. Finally, the paper is concluded with a summary and suggestions for future developments in Section V.

II. RELATED WORKS

Based on the technical device, CI test designs can be practically clustered into four main groups: distance-based methods [39], [8], [41], kernel-based methods [10], [46], [7], [38], regression-based methods [43], and lastly model-based methods [29], [3], [21], [35].

A. Distance-based methods

Starting from the most common definition of conditional independence—$X \perp Y \mid Z$ if and only if $p(x \mid z)p(y \mid z) = p(x,y \mid z)$ (or equivalently, $p(x \mid y,z) = p(x \mid z)$) for every realizations $y$ and $z$ of $Y$ and $Z$, respectively—early methods set the first building blocks by explicitly estimating and comparing the relevant densities or distributions.

For example, [39] measure the distance between two conditionals $p(X \mid y,z)$ and $p(X \mid z)$ using the weighted Hellinger distance. Following this direction, [8] devise a new conditional dependence measure equal to the supremum of the Wasserstein distance between $p(X \mid y,z)$ and $p(X \mid y',z)$ over all realizations $y,y',z$.

Additionally, in [41] the Wasserstein distance between two conditional distributions $p(X,Y \mid z)$ and $p(X \mid z) \otimes p(Y \mid z)$ is measured for each discretized value of $z$.

B. Kernel-based methods

Many other approaches avoid the difficulties in estimating conditional densities with alternative characterizations of conditional independence. Particularly, when $X,Y,Z$ are jointly multivariate normal then the conditional independence $X \perp Y \mid Z$ reduces to the vanish of the partial correlation coefficient $\rho_{XY,Z}$ [2], which is easy to test for zero since its Fisher transformation follows an approximately normal distribution under the null [13].

Departing from that, a large body of works has focused on kernel methods [10], [46], [7], [38], which can be perceived as a non-parametric generalization of the connection between partial uncorrelatedness and conditional independence of Gaussian variables [46]. These methods follow the CI characterization established in [9] where the conditional independence is expressed in terms of conditional cross-covariance operators of functions in the reproducing kernel Hilbert spaces (RKHS): $\Sigma_{Y \mid Z} \Sigma_{X \mid Z} := \Sigma_{Y \mid Z} - \Sigma_{Y \mid Z} \Sigma_{X \mid Z}^{-1} \Sigma_{Z \mid X}$ where the cross-covariance operator is defined as $\langle g, \Sigma_{Y \mid Z} \rangle := \mathbb{E}_{XY} f(X)g(Y) - \mathbb{E}_X [f(X) \mathbb{E}_Y g(Y)]$ with $f,g$ being respectively functions in RKHS of $X$ and $Y$. This can be interpreted as the generalization of the conventional partial covariance.

In what follows, conditional independence is achieved if and only if the conditional cross-covariance is zero. For this reason, in [10] the Hilbert-Schmidt norm of the partial cross-covariance is tested against zero for the null hypothesis.

C. Regression-based methods

Regression-based CI tests [45], [44], [43] assume that $Z$ is a confounder set of $X$ and $Y$, as well as the relationships between $Z$ and $X/Y$ are additive noise models (i.e., $X := f(Z) + E$, $Z \perp \perp E$). Therefore, by the use of a suitable regression function, we can remove all the information from $Z$ embedded in $X/Y$ by simply subtracting the regression function, i.e., $r_X := X - f(Z)$ and $r_Y := Y - \hat{g}(Z)$. After these procedure, the conditional independence $X \perp Y \mid Z$ can be simplified to $r_X \perp r_Y$. Alternatively, in [12] the hypothesis testing problem $X \perp Y \mid Z$ is converted into $X - f(Z) \perp (Y,Z)$. Meanwhile, the problem is transformed into testing for $X - f(Z) \perp (Y - \hat{g}(Z), Z)$ in [45].

Nonetheless, the assumptions required by regression-based methods are relatively strong overall. As proven in [14], in general, we can only obtain residuals independent of $Z$ if regression is performed against the true “cause” in the data generating process, i.e., if data is generated as $Z := f(X) + E$, $X \perp \perp E$ then $X - \mathbb{E}[X \mid Z]$ typically still depends on $Z$. To see why, let $Z := \sqrt{X} + E$, $E \sim N(0,1)$, then $X - \mathbb{E}[X \mid Z] = E^2 - 2EZ^2 - 1$ still statistically depends on $Z$.

Additionally, the additive noise model assumption is also easy to be violated. If the generating process involves non-additive noises then the regression residuals can still be dependent on $Z$, making the equivalence $X \perp Y \mid Z \Leftrightarrow r_X \perp r_Y$ invalid. For example, if $X := f(Z) \times E$, $E \sim N(0,1)$ then $X - \mathbb{E}[X \mid Z] = f(Z) \times E$ which is still dependent on $Z$.

D. Model-based approaches

Apart from the aforementioned methods, model-based approaches more heavily borrow supervised and unsupervised learning algorithms as the basis. For instance, recently GANs have been employed [3], [35] to implicitly learn to sample from the conditionals $p(X \mid Z)$ and $p(Y \mid Z)$.

In [3] the main motivation is that for any dependence measure $\rho$ and $\hat{X} \sim p(X \mid Z)$ with $Y \perp \perp \hat{X}$, under both hypotheses, $\rho(X,Y,Z)$ should be at least $\rho(\hat{X},Y,Z)$ and the equality occurs only under $H_0$. This key observation motivates the authors to employ GANs to learn the generator for $p(X \mid Z)$. Then, the test’s $p$-value can be empirically estimated by repeatedly sampling $\hat{X}$ and calculating the dependence measure without any knowledge of the null distribution. Similarly, the double GAN approach [35] goes one step further—two generators are used in order to learn both $p(X \mid Z)$ and $p(Y \mid Z)$, then the test statistics is calculated.
as the maximum of the generalized covariance measures of multiple transformation functions.

Differently from those, since conditional independence coincides with zero conditional mutual information (CMI), which is a natural and well-known measure of conditional dependence, many methods aim to estimate CMI as the test statistics [29], [21], [18]. In [29], the CMI is estimated via several $k$-NN entropy estimators [17] and the test statistics is empirically estimated by randomly shuffling samples of $X$ in a way that preserves $p(X \mid Z)$ while breaking the conditional dependence between $X$ and $Y$ given $Z$.

As an extension to [29], since $k$-NN CMI estimators are erroneous in high dimensions which is followed by the failed tests, in [18] CMI is replaced with the short expansion of CMI, computed via the Möbius representation of CMI, which offers simple asymptotic null distributions that allow for an easier construction of the conditional independence test. Additionally, [21] propose a classifier-based estimator for the Kullback-Leibler divergence to measure the divergence of $p(X, Y \mid Z)$ and $p(X \mid Z) \otimes p(Y \mid Z)$, which is essentially CMI.

Following a slightly similar approach, the classification-based CI test [34] reduces the CI testing problem into a binary classification problem, where the central idea is that under the null hypothesis, a binary classifier cannot differentiate between the original dataset and a shuffled dataset that forces the conditional independence $X \perp \!\!\!\!\perp Y \mid Z$; whereas the difference under the alternative hypothesis can be easily captured by the classifier.

E. Our approach

Our LCIT method departs from regression-based methods in the sense that it does not require any of the limited assumptions supposed by these methods. More particularly, we devise a “generalized residual”, referred to as a “latent representation”, such that it is independent from $Z$ without assuming $Z$ is a confounder of $X$ and $Y$ nor the relationships are additive noise models.

Moreover, while our method employs generative models, it approaches the CI testing problem from an entirely different angle—instead of learning to generate randomized samples as in GAN-based methods [3], [35], we explicitly learn the deterministic inner representations of $X$ and $Y$ through invertible transformations of NFs, so that we can directly check for their independence instead of adopting bootstrapping procedures.

III. LATENT REPRESENTATION BASED CONDITIONAL INDEPENDENCE TESTING

Let $X, Y \in \mathbb{R}$ and $Z \in \mathbb{R}^d$ be our random variables and vectors where we wish to test for $X \perp \!\!\!\!\perp Y \mid Z$ and $d$ is the number of dimensions of $Z$. In regard of $X$ and $Y$ being limited to scalars instead of vectors, this is due to the fact that in the majority of applications of conditional independence testing, which include causal discovery tasks, we typically care about the dependence of each pair of univariate variables given other variables. Additionally, according to the Decomposition and Union rules of the probabilistic graphoids [25], the conditional independence between two sets of variables given the third set of variables can be factorized into a series of conditional independencies between pairs of univariate variables. Therefore, for simplicity, this work focuses on real-valued $X$ and $Y$ exclusively.

A. A New Characterization of Conditional Independence

We start by giving the fundamental observation that drives the development of our method:

**Lemma 1.** Assuming there exists random variables $\epsilon_X, \epsilon_Y$ statistically independent of $Z$ and invertible functions (w.r.t. the first argument) $f, g$ such that $X = f(\epsilon_X, Z), \epsilon_X = f^{-1}(X, Z)$ and $Y = g(\epsilon_Y, Z), \epsilon_Y = g^{-1}(Y, Z)$, then

$$X \perp \!\!\!\!\perp Y \mid Z \iff \epsilon_X \perp \!\!\!\!\perp \epsilon_Y$$

**Proof.** Since $f$ and $g$ are invertible, by the change of variables rule we have:

$$p(x \mid z) = p(\epsilon_X \mid z) \left| \frac{\partial f}{\partial \epsilon_X} \right|^{-1} = p(\epsilon_X) \left| \frac{\partial f}{\partial \epsilon_X} \right|^{-1}$$
$$p(y \mid z) = p(\epsilon_Y \mid z) \left| \frac{\partial g}{\partial \epsilon_Y} \right|^{-1} = p(\epsilon_Y) \left| \frac{\partial g}{\partial \epsilon_Y} \right|^{-1}$$
$$p(x, y \mid z) = p(\epsilon_X, \epsilon_Y \mid z) \det \left( \frac{\partial f}{\partial \epsilon_X} \frac{\partial g}{\partial \epsilon_Y} \right)^{-1}$$
$$= p(\epsilon_X, \epsilon_Y) \left| \frac{\partial f}{\partial \epsilon_X} \frac{\partial g}{\partial \epsilon_Y} \right|^{-1}$$

where we ignore $z$ due to the constraint $(\epsilon_X, \epsilon_Y) \perp \!\!\!\!\perp Z$.

Thus, $p(x \mid z) p(y \mid z) = p(x, y \mid z)$ if and only if $p(\epsilon_X) p(\epsilon_Y) = p(\epsilon_X, \epsilon_Y)$, rendering $\epsilon_X$ and $\epsilon_Y$ marginally independent.

For this reason, to test for $X \perp \!\!\!\!\perp Y \mid Z$ we can instead test for $\epsilon_X \perp \!\!\!\!\perp \epsilon_Y$, which is progressively less challenging thanks to the reduced conditioning variables.

Furthermore, since $\epsilon_X$ and $\epsilon_Y$ act as contributing factors to $X$ and $Y$ in the supposed generating process without being observed, we refer to them as latent representations of $X$ and $Y$. This is inspired by regression based methods, where the “residuals” are essentially the additive noises in the data generation, and uniquely obtained by subtracting the regression functions to remove all information from $Z$, i.e., $r_X := X - \mathbb{E}[X \mid Z]$ and $r_Y := Y - \mathbb{E}[Y \mid Z]$. As explained in Section II, while residuals are easy to compute, they cannot completely remove all information from $Z$ as intended without restrictive conditions, including additive noise models and $Z$ being a confounder set of both $X$ and $Y$. Consequently, the dependence between $r_X$ and $r_Y$, which is possibly caused by the remaining influences from $Z$ to them, may not exactly entail $X \not\!\!\!\!\perp \!\!\!\!\perp Y \mid Z$. In contrary, with the help of NFs, the latent variables in our framework are always constructible without
any assumption about the relationship between $Z$ and $X/Y$, thus generalize beyond the regression residuals.

We note that when $p(x \mid z)$ and $p(y \mid z)$ are smooth and strictly positive then the use of the cumulative distribution functions (CDF) $\epsilon_X := F(x \mid z)$, $\epsilon_Y := F(y \mid z)$, $f := F^{-1}(\epsilon_X \mid z)$, and $g := F^{-1}(\epsilon_Y \mid z)$ is naturally a candidate for (1). Notably, the cumulative distribution functions for the alternative unconditional test has also been employed in [26], where quantile regression is used to estimate the cumulative distribution functions. However, in this study, Lemma 1 emphasizes the application of a more generic invertible transformation that is not restricted to CDFs, which can be parametrized with NFs.

**B. Conditional Normalizing Flows for Latent Variable Inference**

In this sub-section we explain in detail the conditional normalizing flows (CNF) models used to infer the latent representations of $X$ and $Y$ conditional on $Z$, which will be used for the proxy unconditional test as in (1). For brevity, since the models for $X$ and $Y$ are identically implemented except for their learnable parameters, we only describe the CNF module for $X$ and the module for $Y$ follows accordingly.

1) *Unconditional Normalizing Flows Modeling:* Normalizing Flows have been progressively developed in the last decade since they were defined in [40] and made popular in [28], [6]. For LCIT, we demonstrate the usage of CDF flows [22] thanks to their simplicity and expressiveness. However, it should be noted that any valid alternative NFs can be naturally adapted into our solution.

The essence of CDF flows begins with the observation that the CDF of any strictly positive density function (e.g., Gaussian, Laplace, or Student’s $t$ distributions) is differentiable and strictly increasing, hence the positively weighted combination of any set of these distributions is also a differentiable and strictly increasing function, which entails invertibility. This allows us to parametrize the flow transformation in terms of a mixture of Gaussians, which is known as a universal approximator of any smooth density [11]. Therefore, we can approximate any probability density function to arbitrary non-zero precision, given a sufficient number of components.

More concretely, starting with an unconditional Gaussian mixture based NF, we denote $k$ as the number of components, along with $\{\mu_i, \sigma_i\}_{i=1}^k$ and $\{w_i\}_{i=1}^k$ as the parameters and the weight for each component in the mixture of univariate Gaussian densities $p(x) = \sum_{i=1}^k w_i \mathcal{N}(x; \mu_i, \sigma_i^2)$, where $w_i \geq 0, \sum_{i=1}^k w_i = 1$. Subsequently, the invertible mapping $\mathbb{R} \mapsto (0, 1)$ is defined as

$$ u(x) = \sum_{i=1}^k w_i \Phi(x; \mu_i, \sigma_i^2) $$

(2)

where $\Phi(x; \mu, \sigma)$ is the cumulative distribution function of $\mathcal{N}(\mu, \sigma)$.

Along with the fact that $u \in (0, 1)$, this transformation entails that $u$ has a standard uniform distribution:

**Algorithm 1:** The latent inference algorithm.

**Input:** Empirical samples $D = \{(x_i, z_i)\}_{i=1}^n$ of $(X, Z)$ as well as additional hyper-parameters for training, for example the learning rate $\eta$.

**Output:** The corresponding latents $\epsilon_X$ of $X$ given $Z$.

1) Initialize neural networks $\text{MLP}_\mu$, $\text{MLP}_{\log \sigma^2}$, and $\text{MLP}_w$. Denote the union set of their parameters as $\theta$.

2) Repeat until converge:

   a) Sample a mini-batch $B$ of $b$ samples from $D$.
   b) Compute the mini-batch means, variances, and weights of the conditional Gaussian mixtures:

   $$ \mu := \text{MLP}_\mu(z_B) $$
   $$ \sigma^2 := \exp(\text{MLP}_{\log \sigma^2}(z_B)) $$
   $$ w := \text{MLP}_w(z_B) $$

   c) Compute the mini-batch log-likelihood:

   $$ \mathcal{L} := \frac{1}{b} \sum_{i \in B} \log \langle w_i, \mathcal{N}(x_i; \mu_i, \sigma_i^2) \rangle $$

   d) Update parameters using gradient ascent:

   $$ \theta := \theta + \eta \nabla_{\theta} \mathcal{L} $$

3) Infer the latents for the whole dataset $D$:

   $$ \mu := \text{MLP}_\mu(z_D) $$
   $$ \sigma^2 := \exp(\text{MLP}_{\log \sigma^2}(z_D)) $$
   $$ w := \text{MLP}_w(z_D) $$
   $$ u := \langle w, \Phi(x_D; \mu, \sigma^2) \rangle $$
   $$ \epsilon_X := \Phi^{-1}(u) $$

4) Return $\epsilon_X$.

$$ p(u) = p(x) \left| \frac{\partial u}{\partial x} \right|^{-1} $$

$$ = p(x) \left| \sum_{i=1}^k w_i \mathcal{N} \left( x; \mu_i, \sigma_i^2 \right) \right|^{-1} $$

$$ = p(x) \left| p(x) \right|^{-1} $$

$$ = 1 $$

(3)

Following this reasoning, the transformation (2) maps a variable $x$ with a Gaussian mixture distribution, which is multimodal and complex, into a simpler standard uniform distribution. Moreover, due to its monotonicity, it is also possible to reverse the process to generate new $x$ after sampling $u$, though it is not necessary in the considering application of CI testing.

2) *From Unconditional to Conditional Normalizing Flows:* Next, to extend unconditional NF to conditional NF, we
parametrize the weights, means, as well as variances of the Gaussian components as functions of \( z \) using neural networks. To be more specific, we parametrize \( \mu (z) \in \mathbb{R}^k \) as a simple Multiple Layer Perceptron (MLP) with real-valued outputs. As for \( \sigma^2 \), since it is constrained to be positive, we instead model \( \log \sigma^2 (z) \in \mathbb{R}^k \) with an MLP, similarly as \( \mu (z) \).

Finally, for the weights, which must be non-negative and sum to one, \( w_i (z) \in (0, 1)^k \) is parametrized with an MLP with the Softmax activation function for the last layer. These steps can be summarized as follows:

\[
u (x, z) := \sum_{i=1}^{k} w_i (z) \Phi \left( x; \mu_i (z), \sigma_i^2 (z) \right)
\]

It is worth emphasizing that this translation naturally preserves the property similarly to (3). In another word, \( u (x, z) \in (0, 1) \) and

\[p (u \mid z) = p (x \mid z) \left| \frac{\partial u}{\partial x} \right|^{-1} = 1 \]

\[p (u) = \int p (u \mid z) p (z) dz = \int p (z) dz = 1\]

Therefore, \( U \) is both conditionally and marginally standard uniform regardless of the value of \( z \), making \( \hat{U} \) unconditionally independent of \( Z \).

Moreover, we introduce an additional flow that depends on \( u \) only. This flow adopts the inverse cumulative distribution function (iCDF) of the standard Gaussian distribution, to transform \( U \) from a standard uniform variable to a standard Gaussian variable, which is the final “latent” variable we use for the surrogate test in (1):

\[
\epsilon (u) := \Phi^{-1} (u; 0, 1)
\]

3) Learning Conditional Normalizing Flows: Similarly to conventional NFs, we adopt the Maximum Likelihood Estimation (MLE) framework to learn the CNF modules for \( X \) and \( Y \).

With a fixed number of components \( k \), we denote \( \theta \) as the total set of parameters to be learned, which includes the parameters of the neural networks \( \mu (z) \), \( \log \sigma^2 (z) \), and \( w (z) \). Then, the conditional likelihood of \( X \) is given by

\[
p_\theta (x \mid z) = \sum_{i=1}^{k} w_i (z) \mathcal{N} \left( x; \mu_i (z), \sigma_i^2 (z) \right)
\]

and we aim to maximize the log-likelihood of observed \( X \) conditioned on \( Z \) over the space of \( \theta \):

\[\mathcal{L} (\theta) := \frac{1}{n} \sum_{i=1}^{n} \log p_\theta (x_i \mid z_i)\]

\[\theta_{\text{MLE}} := \arg \max_{\theta} \mathcal{L} (\theta)\]

where \( \{(x_i, z_i)\}_{i=1}^{n} \) is the set of \( n \) observed samples of \( (X, Z) \).

Algorithm 2: The proposed Latent representation based Conditional Independence Testing (LCIT) algorithm.

**Input:** Empirical samples \( \mathcal{D} = \{(x_i, y_i, z_i)\}_{i=1}^{n} \) of \( (X, Y, Z) \) and the significance level \( \alpha \).

**Output:** The p-value and whether \( X \perp Y \mid Z \) or not.

1) Use Algorithm 1 to infer the latents \( \epsilon_X \) and \( \epsilon_Y \).
2) Calculate the test statistic and p-value:

\[r := \frac{\text{cov} (\epsilon_X, \epsilon_Y)}{\sigma_{\epsilon_X} \sigma_{\epsilon_Y}} \]

\[t := \frac{1}{2} \ln \frac{1 + r}{1 - r} \]

\[p\text{-value} := 2 \left( 1 - \Phi \left( |t| \sqrt{n - 3} \right) \right)\]

3) Return p-value and

Conclusion: \( X \perp Y \mid Z \) if p-value > \( \alpha \)

\( X \not\perp Y \mid Z \) if p-value \( \leq \alpha \)

Subsequently, a gradient based optimization framework can be applied to learn \( \theta \) since \( \mathcal{L} \) is fully differentiable. In summary, Algorithm 1 highlights the main steps of the training process.

C. Marginal Independence Test for the Latents

For two jointly Gaussian variables, their independence is equivalent to zero Pearson’s correlation coefficient.\(^2\) Therefore, we can resort to Fisher’s transformation to get the test statistics, which has approximate Gaussian distribution under the null hypothesis, hence the closed form of the p-value is available [13].

To be more specific, first we calculate the Pearson’s correlation coefficient \( r \) between \( \epsilon_X \) and \( \epsilon_Y \), then turn it into the test statistic \( t \) using the Fisher’s transformation:

\[r := \frac{\text{cov} (\epsilon_X, \epsilon_Y)}{\sigma_{\epsilon_X} \sigma_{\epsilon_Y}} \]

\[t := \frac{1}{2} \ln \frac{1 + r}{1 - r} \]

where the test statistic \( t \) has an approximate Gaussian distribution with mean \( \frac{1}{2} \ln \left( \frac{1 + r}{1 - r} \right) \) and standard deviation of \( \frac{1}{\sqrt{n - 3}} \) where \( r \) is the true correlation between \( \epsilon_X \) and \( \epsilon_Y \), and \( n \) is the sample size.

Therefore, under the null hypothesis where \( r = 0 \), the p-value for \( t \) can be calculated as:

\[p\text{-value} := 2 \left( 1 - \Phi \left( |t| \frac{1}{\sqrt{n - 3}} \right) \right)\]

Finally, with a significance level of \( \alpha \), the null hypothesis \( H_0 \) is rejected if p-value < \( \alpha \), otherwise we fail to reject \( H_0 \)

\(^2\)While our procedure only constrains \((\epsilon_X, \epsilon_Y)\) to be marginally Gaussian, the experiments show that it is still robust in a wide range of scenarios.
Figure 2: Hyper-parameter tuning results for (a) the number of mixture components and (b) hidden layer size. The number in each cell denotes the number of runs that have the respective configuration as the best setting recorded. Each column sums to 50 independent runs.

and have to conclude conditional dependence \( X \perp Y \mid Z \). To summarize, see Algorithm 2 for the whole computation flow of the proposed LCIIT method.

IV. EXPERIMENTS

A. Setup

1) Methods: We demonstrate the effectiveness of the LCIIT in conditional independence testing tasks on synthetic and real data against popular and recent state-of-the-art methods across different approaches. More specifically, we consider the Kernel-based KCIT\(^3\) method [46] as a popular competitor, the recently emerged residual similarity based SCIT\(^4\) approach [43], and lastly the classification based CCIT\(^5\) algorithm [34]. Regarding the configurations, we use the default parameters recommended by respective baseline methods. Furthermore, while CCIT offers hyper-parameters selection as is, the KCIT implementation does not provide any such procedure.

Additionally, for all methods, we first apply a standard normalization step for each of \( X, Y, \) and \( Z \) before performing the tests.

Specifically for LCIIT, we parametrize MLP\(_{\mu}\), MLP\(_{\log \sigma^2}\), and MLP\(_{\nu}\) with neural networks of one hidden layer, Rectifier Linear Unit (ReLU) and Batch-normalization [16] activation functions. The hyper-parameters specifications and analyses are considered in the followings.

2) Training CNFs: We implement the CNF modules using the PyTorch framework [23]. Each CNF module is trained using the Adam optimization algorithm with fixed learning rate of \( 5 \times 10^{-3} \), weight decay of \( 5 \times 10^{-5} \) to help regularize the model’s complexity, and batch size of 64.

3) Data processing: Before feeding data into the CNF modules, apart from data standardization as other methods, we additionally handle outliers by clipping the data to be in between the 2.5% and 97.5% quantiles of each dimension, which helps stabilize the training process since neural networks can be very sensitive to extreme values.

Subsequently, the input dataset is divided into training and validation sets with a ratio of 70/30, where the training portion is used to learn parameters and the validation set enables early stopping. We notice that typically, the training process only requires under 20 training epochs.

4) Hyper-parameters: The most important hyper-parameters presented in our models are the number of Gaussian mixture components and the hidden layer sizes, which together determine the expressiveness of the CNF. To examine which set of configuration works best, we furthermore perform hyper-parameter tuning on these two factors using the Optuna framework [1].

Specifically, we simulate 50 random datasets in the same manner as in subsection IV-B, both CI and non-CI labels, for each number of dimensions of \( Z \) varying in \{25, 50, 75, 100\}. With each dataset we execute 20 Optuna trials to find the best configuration, where the number of components varies in \{8, 16, 32, 64, 128, 256\} and the number of units in the hidden layer takes value in \{4, 8, 16, 32, 64, 128, 256\}. The objective is the sum of the maximum log-likelihoods of \( X \) and \( Y \) conditioned on \( Z \). Finally, the most advantageous setting by far is recorded.

The summary of best configurations found via hyper-parameter tuning is showed in Figure 2. It is clear that the more mixture components is usually preferable, while a small number of hidden units is sufficiently effective to retain a high performance. Based on these, we fix 32 Gaussian components for all other experiments in order to keep computations low with only a small loss of performance compared with larger numbers of components. On another hand, four hidden units is also used for every experiments since it is both computationally efficient and sufficiently expressive.

B. Synthetic data

Following several closed related studies [46], [7], [38], [3], we randomly simulate the datasets following the post-nonlinear additive noise model:

\[
\mathcal{H}_0 : Z := f (X \otimes a + E_f) , \quad Y := g (\langle Z, b \rangle + E_g)
\]

\[
\mathcal{H}_1 : Z := f (X \otimes a + E_f) , \quad Y := g (\langle Z, b \rangle + cX + E_g)
\]

with \( X := 2E_X \) where \( E_X, E_f, \) and \( E_g \) are independent noise variables following the same distribution randomly selected from \( \{ \mathcal{U} (-1,1), \mathcal{N} (0,1), \text{Laplace} (0,1) \} \). The \( \otimes \) and \( \langle \cdot, \cdot \rangle \) denote the outer and inner products, respectively. Additionally, \( a, b \sim \mathcal{U} (-1,1)^d, \quad c \sim \mathcal{U} (1,2), \quad \) and \( f,g \) are uniformly chosen from a rich set of mostly non-linear functions \( \{ ax, x^2, x^3, \tan h x, x^{-1}, e^{-x}, \frac{1}{1+e^{-x}} \}^6 \).

\(^3\)We use the KCIT implementation from the CMU causal-learn package: https://github.com/cmuphila/causal-learn
\(^4\)We follow the authors’ original source code in Matlab: https://github.com/Causality-Inference/SCIT
\(^5\)We use the implementation from original authors: https://github.com/rajatsen91/CCIT

\(^6\)For numerical stability, the input is appropriately scaled and translated before being fed into each function.
Effect of different sample sizes: To study the performance of the LCIT against alternative tests across different sample sizes, we fix the dimensionality $d$ of $Z$ at 25 and vary the sample size from 250 to 1,000. We measure the CI testing performance under four different metrics, namely the $F_1$ score (higher is better), Area Under the Receiver Operating Characteristic Curve (AUC, higher is better), as well as Type I and Type II error rates (lower is better). More specifically, Type I error refers to the proportion of false rejections under $H_0$, and Type II error reflects the proportion of false acceptances under $H_1$. These metrics are evaluated using 250 independent runs for each combination of method, sample size, and label. Additionally, for $F_1$ score, Type I, and Type II errors, we adopt the commonly used significance level of $\alpha = 0.05$.

The result is reported in Figure (3), which shows that our method is the only one achieving good and stable performance in all four evaluation criterions. Remarkably, LCIT scores the highest in terms of $F_1$ measure, surpassing all other tests with clear differences. Furthermore, LCIT, along with KCIT, also obtains the highest AUC scores, approaching closely to 100% as more samples are used, and marginally outperforms the two recent state-of-the-arts CCIT and SCIT at considerable margins. For both Type I and II errors, LCIT stably earns the second lowest in overall, at around 10%.

Meanwhile, KCIT achieves the lowest Type II errors, but its Type I errors are completely larger than those of all other methods, suggesting that KCIT majorly returns conditional dependence as output. In contrary, while CCIT is able to obtain virtually no error in Type I, its use becomes greatly unreliable when viewed from the perspective of Type II errors.
This indicates that CCIT in general usually favors outputting conditional independence as the answer.

2) Effect of high dimensional conditioning sets: In Figure (4) we study the change in performance of LCIT as well as other methods in higher dimensional settings. Concretely, we fix the sample size at 1,000 samples and increase the dimension of $Z$ from 25 to 100. The result shows that our method consistently outperforms other state-of-the-arts as the dimensionality of $Z$ increases, as evidenced by the highest AUC scores in overall, leaving CCIT and SCIT by up to roughly 40 units, while having comparably low error rates.

Generally, we can see a visible decline in performance of all methods, especially KCIT and CCIT. The AUC score of KCIT drops rapidly by 20 units from the smallest to largest numbers of dimensions, whereas its $F_1$ score deteriorates quickly to half of the initial value, and the Type I errors are always the highest among all considered algorithms. On another hand, CCIT also has vanishing Type I errors but exceedingly high Type II errors similarly to that in Figure (3).

C. Real data

To furthermore demonstrate the robustness of the proposed LCIT test, we evaluate it against other state-of-the-arts in CI testing on real datasets.

In general, real datasets of triplets $(X, Y, Z)$ for CI test benchmarking are not available, so we have to resort to data coming with ground truth networks instead, which are still relatively rare and there are few consensus benchmark datasets.

In this study, we examine two datasets from the Dialogue for Reverse Engineering Assessments and Methods challenge$^7$, ninth edition (referred to as DREAM4) [20], [19], where the data is publicly accessible with the ground-truth gene regulatory networks presented. The challenge’s objective is to recover the gene regulatory networks given their gene expression data only. Therefore, the data sets are well fit to the application of our method and CI tests in general.

Regarding data description, each data set includes a ground truth transcriptional regulatory network of *Escherichia coli* or *Saccharomyces cerevisiae*, along with observations of gene expression measurements. We denote the two considered datasets as D4-A and D4-B, where D4-A is from the first sub-challenge of the contest that contains 10 genes with 105 gene expression observations, whereas D4-B comes from the second sub-challenge and consists of 100 genes complemented with 210 gene expression samples.

Next, we extract conditional independent and conditional dependent triplets $(X, Y, Z)$ from the ground truth networks. This process is done based on the fact that if there is a direct connection between two nodes in a network, then regardless of the conditioning set, they remain conditionally dependent. Otherwise, the union of their parent sets should be separate all paths connecting them, rendering them conditionally independent given the joint parents set [24]. In short, if there is an edge between $X$ and $Y$ in the ground truth network, we add to the data set $\{(X, Y, Z_i)\}_{i=1}^5$ where $Z_i$ is a random subset of the remaining nodes with size $d - 4$; otherwise we add $(X, Y, \text{Parents}(X) \cup \text{Parents}(Y))$ to the data set. Finally, to create class-balance datasets, for D4-A, we sample 30 conditional independence and 30 conditional dependence relationships from the created data set, while the number of relationships from D4-B are 50 each.

The CI testing performance on the DREAM4 datasets is reported in Figure 5. It can be seen that the results follow relatively consistently with synthetic data scenarios, with LCIT being the best performer, followed by KCIT. Meanwhile, CCIT and SCIT considerably underperform with AUC scores around or under 50%, comparable to a fair-coins random guesser.

V. CONCLUSION AND FUTURE WORK

In this paper we propose a representation learning approach to conditional independence testing called LCIT. Through the use of conditional normalizing flows, we transform the difficult conditional independence testing problem into an easier unconditional independence testing problem. We showcase the performance of our LCIT method via intensive experiments including synthetic datasets of highly complex relationships, as well as real datasets in bio-genetics. The empirical results show that LCIT performs really well and is able to consistently outperform existing state-of-the-arts.

Conditional independence testing is a generic tool that serves as the basis of a wide variety of scientific tasks, especially in causal discovery. Therefore, the development of LCIT offers a promising generic alternative solution for these problems and methods.

As for future perspectives, since the latent representation based approach is first used in LCIT, it opens doors for further scientific developments of conditional independence tests based on representation learning, which are expected to greatly improve from LCIT and are able to extend to more challenging scenarios such as heterogeneity and missing data.

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