Learning to Induce Causal Structure

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Abstract

The fundamental challenge in causal induction is to infer the underlying graph structure given observational and/or interventional data. Most existing causal induction algorithms operate by generating candidate graphs and then evaluating them using either score-based methods (including continuous optimization) or independence tests. In this work, instead of proposing scoring function or independence tests, we treat the inference process as a black box and design a neural network architecture that learns the mapping from both observational and interventional data to graph structures via supervised training on synthetic graphs. We show that the proposed model generalizes not only to new synthetic graphs but also to naturalistic graphs.

1 Introduction

The problem of discovering the causal relationships that govern a system through observing its behavior, either passively (observational data) or by manipulating some of its variables (interventional data), lies at the core of many scientific disciplines, including medicine, biology, and economics. By using the graphical formalism of causal Bayesian networks (CBNs) Koller & Friedman (2009); Pearl (2009), this problem can be framed as inducing the graph structure that best represents the relationships. Most approaches to causal structure induction are based on an unsupervised learning paradigm in which the structure is directly inferred from the system observations, either by ranking different structures according to some metrics (score-based approaches) or by determining the presence of an edge between pairs of variables using conditional independence tests (constraint-based approaches) Drton & Maathuis (2017); Heinze-Deml et al. (2018a,b); Glymour et al. (2019); Ke et al. (2020a) (see Fig. 1(a)). The unsupervised paradigm poses however some challenges: score-based approaches are burdened with the high computational cost of having to explicitly consider all possible structures and with the difficulty of devising metrics that can balance fit to the data with constraints for differentiating causal from a purely statistical relationships (e.g. sparsity of the structure or simplicity of the generation mechanism); constraint-based methods are sensitive to failure of independence tests and require faithfulness, a property that does not hold in many real-world scenarios Koski & Noble (2012); Mabrouk et al. (2014).

In this work, we propose a supervised learning paradigm in which a model is first trained on synthetic data generated using different CBNs to learn a mapping from data to graph structures and then used to induce the structures underlying datasets of interests (see Fig. 1(b)). The model is a novel variant of a transformer neural network that receives as input a dataset consisting of observational and interventional samples corresponding to the same CBN and outputs a prediction of the CBN graph structure. The mapping from the dataset to the underlying structure is achieved through an attention mechanism which alternates between attending to different variables in the graph and to different samples from a variable. The output is produced by a decoder mechanism that operates as

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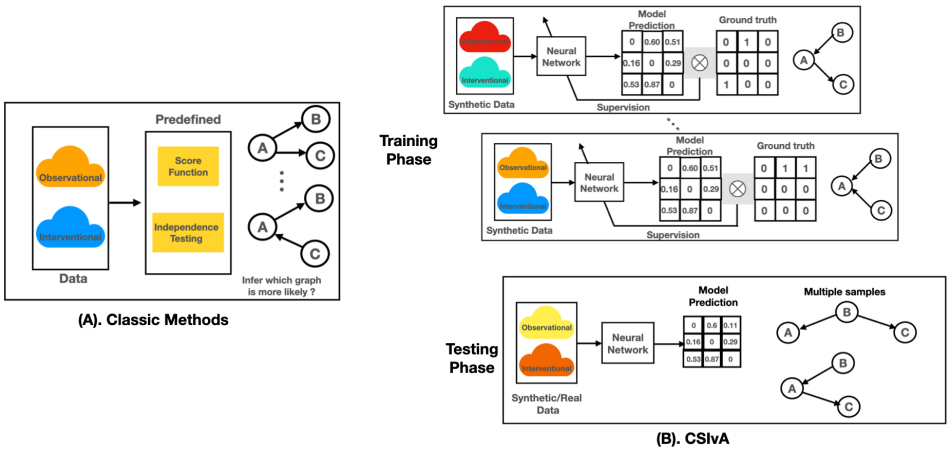


Figure 1: (A). Standard unsupervised approach to causal structure induction: Algorithms use a predefined scoring metric or statistical independence tests to select the best candidate structures. (B). Our supervised approach to causal structure induction (CSIvA): A model is presented with data and structures as training pairs and learns a mapping between them.

an autoregressive generative model on the inferred structure. The proposed approach can be viewed as a form of meta-learning, as the model learns about the relationship between datasets and structures underlying them. Supervised learning methods based on observational data have been shown to be feasible by Lopez-Paz et al. (2015a,b) and Li et al. (2020). By allowing the use of both observational and interventional data, the proposed method enables greater flexibility.

A requirement of a supervised approach would seem to be that the distributions of the training and test data match or highly overlap. Obtaining real-world training data with a known causal structure that matches test data from multiple domains is extremely challenging. We show that meta-learning enables the model to generalize well to data from naturalistic CBNs even if trained on synthetic data with relatively few assumptions. We show that the proposed model can learn a mapping from datasets to structures and outperform unsupervised approaches on classic benchmarks such as the Sachs (Sachs et al., 2005) and Asia (Lauritzen & Spiegelhalter, 1988) datasets, despite never directly being trained on such data. Our contributions can be summarized as follows:

- We tackle causal structure induction with a supervised approach (CSIvA) that maps datasets composed of both observational and interventional samples to structures.
- We introduce a variant of a transformer architecture whose attention mechanism is structured to discover relationships among variables across samples.
- We show that CSIvA generalizes to novel structures, whether or not training and test distributions match. Most importantly, training on synthetic data transfers effectively to naturalistic CBNs.

2 Background

In this section we give some background on causal Bayesian networks (CBNs) and on transformer neural networks, which form the main ingredients of CSIvA (more details are given in Appendix A). **Causal Bayesian networks.** A *Bayesian network* (Pearl, 1988; Cowell et al., 2007; Koller & Friedman, 2009; Pearl, 2009) is a pair $\mathcal{M} = \langle \mathcal{G}, p \rangle$, where $\mathcal{G}$ is a *directed acyclic graph* (DAG) whose nodes $X_1, \ldots, X_N$ represent random variables and edges express statistical dependencies among them, and where p is a joint distribution over all nodes that factorizes into the product of the conditional probability distributions (CPDs) of each node X_n given its *parents* $\text{pa}(X_n)$ (namely all nodes with an edge onto X_n), i.e. $p(X_1, \ldots, X_N) = \prod_{n=1}^{N} p(X_n \,|\, \text{pa}(X_n))$. The structure of $\mathcal{G}$ can be represented by an adjacency matrix A, defined by setting the (k, l) entry, $A_{k,l}$, to 1 if there is an edge from X_l to X_k and to 0 otherwise. Therefore, the n-th row of A, denoted as $A_{n,:}$, indicates the

parents of X_n while the n-th column, denoted as $A_{:,n}$, indicates the *children* of X_n. A BN $\mathcal{M}$ can be given causal semantic by interpreting an edge between two nodes as expressing causal rather than statistical dependence. For the experiments, we consider datasets whose elements are *observational data samples*, namely samples from $p(X_1, \ldots, X_N)$, and *interventional data samples*, namely samples from $p_{\text{do}(X_{n'}=x)}(X_1, \ldots, X_N) = \prod_{n=1, n\neq n'}^{N} p(X_n \mid \text{pa}(X_n))\delta_{X_{n'}=x}$, where $\delta_{X_{n'}=x}$ is a delta function, corresponding to an *atomic intervention* on variable $X_{n'}$ that forces the variable to take on value x. Two adjacency matrices A^i and A^j can be compared using the *Hamming distance* ($\mathcal{H}$), defined as the norm of the difference between them, $\mathcal{H} = |A^i - A^j|_1$.

Transformer neural network. A transformer Vaswani et al. (2017); Devlin et al. (2018) is a neural network equipped with layers of self-attention mechanisms that make them well suited to modelling structured data. In traditional applications of transformers, attention is used to account for the sequential nature of the data, such as e.g. for a sentence being a stream of words. In CSIvA, each input of the transformer is a dataset of observational or interventional samples corresponding to the same CBN, the attention is used to account for the structure induced by the CBN graph structure and by having different samples from the same node. Transformers are permutation invariant with respect to the positions of the input elements, which ensures that the prediction of a graph structure does not depend on the node and sample position.

3 Causal Structure Induction via Attention (CSIvA)

The proposed approach is to treat causal structure induction as a supervised learning problem, by training a neural network to learn to map observational and interventional data to the graph structure of the underlying CBN. Obtaining diverse, real-world, data with known causal relationships in amounts sufficient for supervised training is not feasible. The key contribution of this work is to introduce a method that uses synthetic data generated from CBNs with different graph structures and CPDs that is robust to shifts between the training and test data distributions.

3.1 Supervised approach

The proposed approach is to learn a distribution of graphs conditioned on observational and interventional data as explained below.

We generate training data from a joint distribution $t(\mathcal{G}, \mathcal{D})$ between a graph $\mathcal{G}$ and a dataset $\mathcal{D}$ comprising of S observational and interventional samples from a CBN associated to $\mathcal{G}$ as follows. We first sample a set of graphs $\{\mathcal{G}^i\}_{i=1}^I$ with nodes $X_1^i, \ldots, X_N^i$ from a common distribution $t(\mathcal{G})$ as described in Section 4.1 (to simplify notation, in the remainder of the paper we omit the graph index i when referring to nodes), and then associate random CPDs to the graphs as described in Section 4.2. This results in a set of CBNs $\{\mathcal{M}^i\}_{i=1}^I$. For each CBN $\mathcal{M}^i$, we then create a dataset $\mathcal{D}^i = \{x^s\}_{s=1}^S$, where each element $x^s := (x_1^s, \ldots, x_N^s)^\mathsf{T}$ is either an observational data sample or an interventional data sample obtained by performing an atomic intervention on a randomly selected node in $\mathcal{G}^i$.

Model definition and training objective. The proposed model defines a distribution $\hat{t}(\mathcal{G} \mid \mathcal{D}; \Theta)$ over graphs conditioned on observation and interventional data and parametrized by Θ. Specifically, $\hat{t}(A \mid \mathcal{D}; \Theta)$ has the following auto-regressive form: $\hat{t}(A \mid \mathcal{D}; \Theta) = \prod_{l=1}^{N^2} \sigma(A_l; \hat{A}_l = f_\Theta(A_{1,\ldots,(l-1)}, \mathcal{D}))$, where $\sigma(\cdot; \rho)$ is the Bernoulli distribution with parameter ρ, which is a function f_Θ built from an encoder-decoder architecture explained in Section 3.2 taking as input previous elements of the adjacency matrix A (represented here as an array of N^2 elements) and $\mathcal{D}$.

Model training. The proposed model is trained via maximum likelihood estimation (MLE), i.e as $\Theta^* = \text{argmin}_\Theta \mathcal{L}(\Theta)$, where $\mathcal{L}(\Theta) = -\mathbb{E}_{(\mathcal{G},\mathcal{D})\sim t}[\ln \hat{t}(\mathcal{G} \mid \mathcal{D}; \Theta)]$, which corresponds to the usual cross-entropy (CE) loss for the Bernoulli distribution. Training is achieved using a stochastic gradient descent (SGD) approach in which each gradient update is performed using a pair $(\mathcal{D}^i, A^i)$. The data-sampling distribution $t(\mathcal{G}, \mathcal{D})$ and the MLE objective uniquely determine the target distribution learned by the model. In the infinite capacity case, $\hat{t}(\cdot \mid \mathcal{D}; \Theta^*) = t(\cdot \mid \mathcal{D})$. To see this, it suffices to note that the MLE objective $\mathcal{L}(\Theta)$ can be written as $\mathcal{L}(\Theta) = \mathbb{E}_{\mathcal{D}\sim t}[\text{KL}(\hat{t}(\cdot \mid \mathcal{D}; \Theta); t(\cdot \mid \mathcal{D}))] + c$,

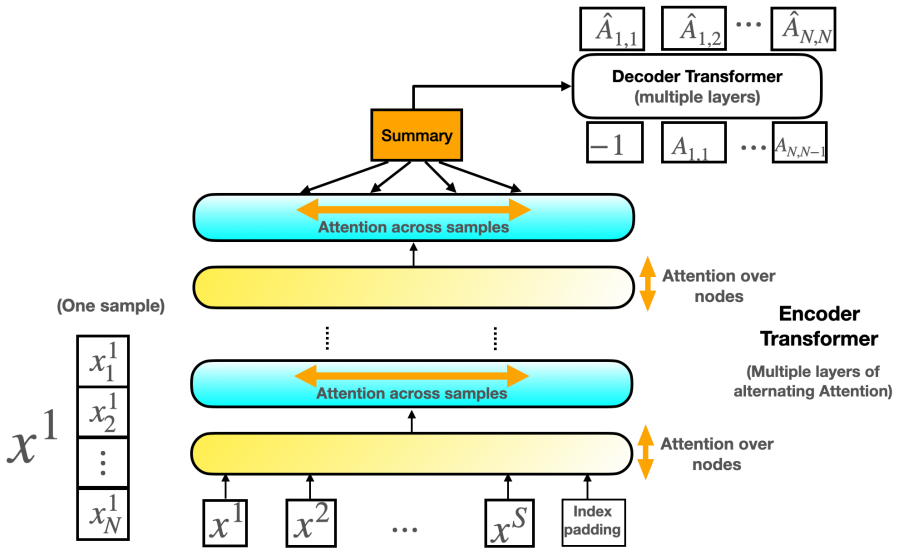


Figure 2: The proposed model architecture and the structure of the input and output at training time. The input is a dataset $\mathcal{D} = \{x^s := (x_1^s, \ldots, x_N^s)^\mathsf{T}\}_{s=1}^S$ of S samples from a CBN and its adjacency matrix A. The output is a prediction $\hat{A}$ of A. Even though the model receives a set of observations $\mathcal{D}$ at each gradient update, this is a single-example SGD approach because each update has only a single target A. The attention in a transformer normally only operates over different columns. We instead also take attention over the different rows, in alternating layers.

where KL is the Kullback-Leibler divergence and c is a constant. In the finite-capacity case, the distribution defined by the model $\hat{t}(\cdot \mid \mathcal{D}; \Theta^*)$ is only an approximation of $t(\cdot \mid \mathcal{D})$.

3.2 Model architecture

The function f_Θ defining the model's probabilities is built using two transformer networks. It is formed by an encoder transformer and by a decoder transformer (which we refer to as "encoder" and "decoder" for short). At training time, the encoder receives as input dataset $\mathcal{D}^i$ and outputs a representation that summarizes the relationship between nodes in $\mathcal{G}^i$. The decoder then recursively outputs predictions of the elements of the adjacency matrix A^i using as input the elements previously predicted and the encoder output. This is shown in Fig. 2 (where with omitted index i, as in the remainder of the section). At test time we obtain deterministic predictions of the adjacency matrix elements by taking the argmax of the Bernoulli distribution and use those as inputs to the decoder.

3.2.1 Encoder

The encoder in the proposed model is structured as an $(N+1) \times (S+1)$ lattice. The $N \times S$ part of the lattice formed by the first N rows and first S columns receives a dataset $\mathcal{D} = \{(x_1^s, \ldots, x_N^s)^\mathsf{T}\}_{s=1}^S$. This is unlike standard transformers which typically receive as input a single data sample (e.g., a sequence of words in neural machine translation applications) rather than a set of data samples. Row $N+1$ of the lattice is used to specify whether each data sample is observational, through value -1, or interventional, through integer value in $\{1, \ldots, N\}$ to indicate the intervened node.

The goal of the encoder is to infer causal relationships between nodes by examining the set of samples. The transformer performs this inference in multiple stages, each represented by one transformer layer, such that each layer yields a $(N+1) \times (S+1)$ lattice of representations. The transformer is designed to deposit its summary representation of the causal structure in column $S+1$.

Embedding of the input. Each data-sample element x_n^s is embedded into a vector of dimensionality H. Half of this vector is allocated to embed the value x_n^s itself, while the other half is allocated to embed the unique identity for the node X_n. The value embedding is obtained by passing x_n^s, whether

discrete or continuous, through an MLP [1] encoder specific to node X_n. We use a node-specific embedding because the values of each node may have very different interpretations and meanings. The node identity embedding is obtained using a standard 1D transformer positional embedding over node indices. For column $S+1$ of the input, the value embedding is a vector of zeros.

Alternating attention. Traditional transformers discover relationships among the elements of a data sample arranged in a one-dimensional sequence. With our two-dimensional lattice, the transformer could operate over the entire lattice at once to discover relationships among both nodes and samples. Given an encoding that indicates the position n, s in the lattice, the model can in principle discover stable relationships among nodes over samples. However, the inductive bias to encourage the model to leverage the lattice structure is weak. Additionally, the model is invariant to sample ordering, which is desirable because the samples are iid. Therefore, we arrange the transformer in CSIvA in alternating layers. In the first layer of the pair, attention operates across all nodes of a single sample $(x_1^s, \ldots, x_N^s)^\mathsf{T}$ to encode the relationships among two or more nodes. In the second layer of the pair, attention operates across all samples for a given node $(x_n^1, \ldots, x_n^S)$ to encode information about the distribution of node values.

Encoder summary. The encoder produces a *summary* vector e_n^{sum} with H elements for each node X_n, which captures essential information about the node's behavior and its interactions with other nodes. The decoder uses this summary information to produce a final graph structure. The summary representation is formed independently for each node and involves combining information across the S samples (the columns of the lattice). This is achieved with a method often used with transformers that involves a weighted average based on how informative each sample is. The weighting is obtained using the embeddings in column $S+1$ to form queries, and embeddings in columns $1, \ldots, S$ to provide keys and values, and then using standard key-value attention.

3.2.2 Decoding the adjacency matrix

The decoder generates a prediction of the adjacency matrix A of the underlying $\mathcal{G}$. It operates sequentially, at each step producing a binary output indicating the prediction $\hat{A}_{k,l}$ of $A_{k,l}$, proceeding row by row. The decoder is an autoregressive transformer, meaning that each prediction $\hat{A}_{kl}$ is obtained based on all elements of A previously predicted, as well as the summary produced by the encoder. CSIvA does not enforce acyclicity. Although this could in principle yield cycles in the graph, in practice we observed strong performance regardless. Nevertheless, one could likely improve the results using post-processing (Lippe et al., 2021) or by extending the method with an accept-reject algorithm (Castelletti & Mascaro, 2022; Li et al., 2022).

Auxiliary loss. We found that autoregressive decoding of the flattened $N \times N$ adjacency matrix is too difficult for the decoder to learn alone. To provide additional inductive bias to facilitate learning of causal graphs, we added the auxiliary task of predicting the parents $A_{n,:}$ and children $A_{:,n}$ of node X_n from the encoder summary, e_n^{sum}. This is achieved using an MLP to learn a mapping f_n, such that $f_n(e_n^{\text{sum}}) = (\hat{A}_{n,:}, \hat{A}_{:,n}^\mathsf{T})$. While this prediction is redundant with the operation of the decoder, it short circuits the autoregressive decoder and provides a strong training signal to support proper training of the decoder.

4 Synthetic data

In this section, we describe how we generated the data from different distributions over BNs structures and CPDs used for training and for testing in Sections 6.1 and 6.2, and for training in Section 6.3.

[1] Using an MLP for a discrete variable is a slightly inefficient implementation of a node value embedding, but it ensures that the architecture is general.

4.1 Graph distribution

We specified a distribution over $\mathcal{G}$ in terms of the number of nodes N (graph size) and number of edges (graph density) present in $\mathcal{G}$. As shown in Zheng et al. (2018); Yu et al. (2019); Ke et al. (2020a), larger and denser graphs are more challenging to learn.

We varied N from 5 to 10. The current implementation of the transformer scales quadratically with N, and therefore does not allow much larger graphs. However, we could readily incorporate transformer architectures that scale linearly with N (Goyal et al., 2021b; Jaegle et al., 2021).

We used the Erdős–Rényi (ER) metric to vary density and evaluated CSIvA on ER-1 and ER-2 graphs, as in Yu et al. (2019); Scherrer et al. (2021). We generated an adjacency matrix A by first sampling a lower-triangular matrix to ensure that it represents a DAG, and by then permuting the order of the nodes to ensure random ordering.

4.2 Conditional probability distributions

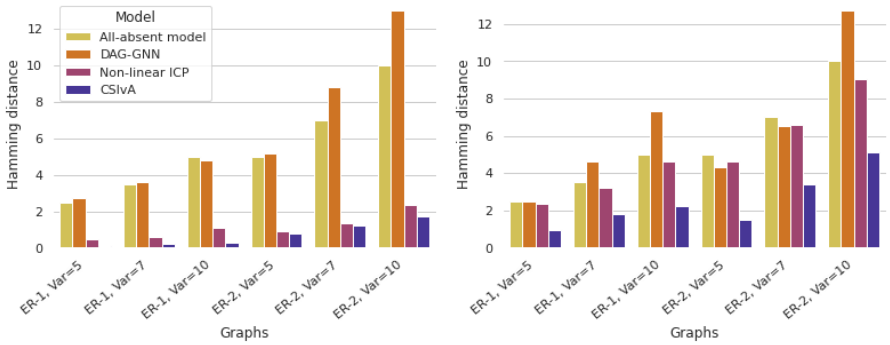
We perform ancestral sampling on the underlying BN. If there is an intervention, it is on a single randomly sampled node (see Section 2). We allow both continuous and discrete nodes.

For continuous nodes with interventions, values are sampled from the uniform distribution $U[-1, 1]$. For ones without interventions, we generated *continuous data* following a similar setup to Zheng et al. (2018) and Yu et al. (2019). Specifically, let X be a $N \times S$ matrix representing S samples of a CBN with N nodes and weighted adjacency matrix A, and let Z be a random matrix of elements in $\mathcal{N}(0, 0.1)$. We generated data as $X_{n,:} = A_{n,:}X + Z_{n,:}$.

For discrete nodes with interventions, values are randomly and independently sampled from $U\{1, \ldots, K\}$ where K indicates the number of categories of the discrete variable. For ones without interventions, we generate discrete data using two different methods: MLP and Dirichlet conditional-probability table generators, which we refer to as *MLP data* and *Dirichlet data*, respectively. The MLP had two fully connected layers of hidden dimensionality 32. Following past work (Ke et al., 2020a; Scherrer et al., 2021), we used a randomly initialized network. The biases were initialized using $U[-0.5, 0.5]$, and the individual weights were initialized using a truncated normal distribution with standard deviation of 1.5. The Dirichlet generator filled in the rows of a conditional probability table by sampling a categorical distribution from a Dirichlet prior with symmetric parameters α. Values of α smaller than 1 encourage lower entropy distributions; values of α greater than 1 provide less information about the causal relationships among variables. We note that this generative procedure is performed prior to node ordering being randomized for presentation to the learning model.

5 Related work

Methods for inferring causal graphs from observational and interventional data can broadly be categorized into score-based (continuous optimization methods included), constraint-based, and asymmetry-based methods. Score-based methods search through the space of possible candidate graphs, usually all DAGs, and ranks them based on some scoring function (Heckerman et al., 1995; Cooper & Yoo, 1999; Chickering, 2002; Tsamardinos et al., 2006; Hauser & Bühlmann, 2012; Goudet et al., 2017; Zhu & Chen, 2019). Recently, Zheng et al. (2018); Yu et al. (2019); Lachapelle et al. (2019) framed the structure search as a continuous optimization problem, which can be seen as a way to optimize for the scoring function. There also exist score-based methods that use a mix of continuous and discrete optimization (Bengio et al., 2019; Ke et al., 2020a; Lippe et al., 2021; Scherrer et al., 2021). Constraint-based methods (Spirtes et al., 2000; Sun et al., 2007; Zhang et al., 2012; Monti et al., 2019; Zhu & Chen, 2019) infer the DAG by analyzing conditional independencies in the data. Eaton & Murphy (2007) use dynamic programming techniques to accelerate Markov Chain Monte Carlo sampling in a Bayesian approach to structure learning for DAGs. Asymmetry-based methods such as Shimizu et al. (2006); Hoyer et al. (2009); Peters et al. (2011); Daniusis et al. (2012); Budhathoki & Vreeken (2017); Mitrovic et al. (2018) assume asymmetry between cause and effect in the data and use this information to estimate the causal structure. Peters et al. (2016);



(a) **Results on continuous data.** (b) **Results on MLP data.**

Figure 3: Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices on the continuous and MLP data, compared to DAG-GNN (Yu et al., 2019) and non-linear ICP (Heinze-Deml et al., 2018a), averaged over 128 sampled graphs. Both non-linear ICP and CSIvA performs well on the easier (linear) continuous data. However, CSIvA significantly outperforms all other baselines on the more challenging MLP data.

Ghassami et al. (2017); Rojas-Carulla et al. (2018); Heinze-Deml et al. (2018a) exploit invariance across environments to infer causal structure. Mooij et al. (2016) propose a modelling framework that leverages existing methods while being more powerful and applicable to a wider range of settings.

Several learning-based methods have been proposed (Guyon, 2013, 2014; Lopez-Paz et al., 2015b; Kalainathan et al., 2018; Goudet et al., 2018; Bengio et al., 2019; Ke et al., 2020a,b). Neural network methods equipped with learned masks exist in the literature (Douglas et al., 2017; Ivanov et al., 2018; Yoon et al., 2018; Li et al., 2019; Goyal et al., 2021a), but only a few have been adapted to causal inference. These works are mainly concerned with learning only one part of the causal induction pipeline, such as learning the scoring function. Therefore, these methods are significantly different from the proposed method, which uses an end-to-end supervised learning approach to learn to map from datasets to graphs. Two supervised learning approaches have been proposed, one framing the task as a kernel mean embedding classification problem (Lopez-Paz et al., 2015a,b) and one operating directly on covariance matrices (Li et al., 2020). Both of these models accept observational data only, and because causal identifiability requires both observational and interventional data, CSIvA is in principle more powerful.

6 Experiments

We report on a series of experiments of increasing challenge to our supervised approach to causal structure induction. First, we examined whether CSIvA generalizes well on synthetic data in the case in which the training and test distributions are identical (Section 6.1). This experiment tests whether the model can learn to map from a dataset to a structure. Second, we examined generalization to an out-of-distribution (OOD) test distribution, and we determined hyperparameters of the synthetic data generating process that are most robust to OOD testing (Section 6.2). Third, we trained CSIvA using the hyperparameters from the second experiment, and evaluated it on a different type of OOD test distribution from two naturalistic CBNs (Section 6.3). This last experiment is the most important test of our hypothesis that causal structure of synthetic datasets can be a useful proxy for discovering causal structure in realistic settings.

Hyperparameters. For all of our experiments (unless otherwise stated) CSIvA was trained on $I = 15,000$ pairs $\{(\mathcal{D}^i, A^i)\}_{i=1}^{I}$, where each dataset $\mathcal{D}^i$ contained $S = 1500$ observational and interventional samples. For experiments on discrete data, a data-sample element x^s could take values in $\{1, 2, 3\}$. Details of the data generating process can be found in Section 4.2. For evaluation in Sections 6.1 and 6.2, CSIvA was tested on $I' = 128$ (different for the training) pairs $\{(\mathcal{D}^{i'}, A^{i'})\}_{i'=1}^{I'}$, where each dataset $\mathcal{D}^{i'}$ contained $S = 1500$ observational and interventional samples. For the Sachs and Asia benchmarks, CSIvA was still tested on $I' = 128$ (different for the training) pairs

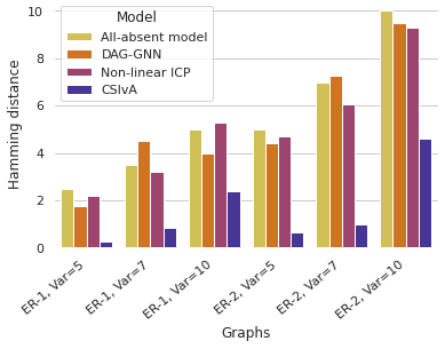


Figure 4: **Results on Dirichlet data**. Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices on the Dirichlet data, averaged over 128 sampled graphs.

$\{(\mathcal{D}^{i'}, A^{i'})\}_{i'=1}^{I'}$, however, $A^{i'} = A^{j'}$ since there is only a single adjacency matrix in each one of the benchmarks.

Each setting of the experiment was run with 3 random seeds. We present test results averaging performance over the 128 datasets and the 3 runs. The model was trained for $500,000$ iterations using the Adam optimizer (Kingma & Ba, 2014) with a learning rate of $1\mathrm{e}{-4}$.

We parameterized CSIvA such that inputs to the encoder were embedded into 128-dimensional vectors. The encoder transformer had 12 layers and 8 attention-heads per layer. The final attention step for summarization had 8 attention heads. The decoder was a smaller transformer with only 4 layers and 8 attention heads per layer. Discrete inputs were encoded using an embedding layer before passing into CSIvA.

Comparisons to baselines. For Section 6.1, we compared CSIvA to two strong baselines in the literature, namely non-linear ICP (Heinze-Deml et al., 2018a) and DAG-GNN (Yu et al., 2019). Non-linear ICP can handle both observational and interventional data, while DAG-GNN can only use observational data. These two baselines are unsupervised methods, i.e., they are not tuned to a particular training dataset but instead rely on a general-purpose algorithm. We also compared to an all-absent model corresponding to a zero adjacency matrix, which acts as a sanity check baseline. We also considered other methods (Chickering, 2002; Hauser & Bühlmann, 2012; Zhang et al., 2012; Gamella & Heinze-Deml, 2020), but only presented a comparison with non-linear ICP and DAG-GNN as these have shown to be strong performing models in other works (Ke et al., 2020a; Lippe et al., 2021; Scherrer et al., 2021). For Section 6.3, we also compared to additional baselines from Chickering (2002); Hauser & Bühlmann (2012); Zheng et al. (2018); Gamella & Heinze-Deml (2020). Note that, methods from Chickering (2002); Zheng et al. (2018); Yu et al. (2019) take observational data only.

DAG-GNN outputs several candidate graphs based on different scores, such as evidence lower bound or negative log likelihood, we chose the best result to compare to CSIvA. Note that non-linear ICP does not work on discrete data, i.e. on the MLP and Dirichlet data, therefore a small amount of Gaussian noise $\mathcal{N}(0, 0.1)$ was added to this data in order for the method to run.

6.1 In-distribution experiments

In this set of experiments, we investigated whether CSIvA can learn to map from data to structures in the case in which the training and test distributions are identical. In this setting, CSIvA (proposed supervised approach) has an advantage over unsupervised ones, as it can learn about the training distribution and leverage this knowledge during testing. We examined the performance on data with increasing order of difficulty, starting with linear (continuous data), before moving to non-linear cases (MLP and Dirichlet data).

Continuous data. Results on continuous data are presented in Figure 3(a). CSIvA achieves Hamming distance $\mathcal{H} < 2$ on all evaluated graphs. Similar to previous findings (Yu et al., 2019; Ke et al., 2020a), larger and denser graphs are more challenging to learn. Non-linear ICP achieves fairly good

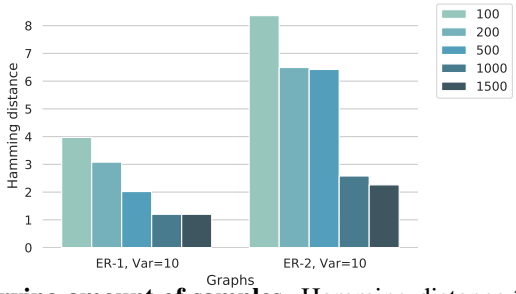


Figure 5: **Results on varying amount of samples**. Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices for synthetic data. Results for CSIvA trained on Dirichlet data with $N = 10$ and $\alpha = 0.5$ with different numbers of samples per CBNs. 1000 samples are sufficient for ER-1 graphs, whereas 1500 samples give a small improvement on ER-2 graphs.

performance, at times approaching that of CSIvA, but required a modification [2] to the dataset wherein multiple samples were collected from the same modified graph after a point intervention (20 samples per intervention), while other methods only sampled once per intervention.

MLP data. Results on MLP data are shown in Figure 3(b). CSIvA significantly outperforms non-linear ICP and DAG-GNN. Differences become more apparent with larger graph sizes ($N = 10$) and denser graphs (ER-2 vs ER-1), as these graphs are more challenging to learn.

Dirichlet data. The Dirichlet data requires setting the values of the parameter α. Hence, we run two sets of experiments on this data.

In the first set of experiments, we investigated how different values of α impact learning in CSIvA. As shown in Table 8 in the appendix, CSIvA performs well on all data with $\alpha \leq 0.5$, achieving $\mathcal{H} < 2.5$ in all cases. CSIvA still performs well when $\alpha = 1.0$, achieving $\mathcal{H} < 5$ on size 10 graphs. Learning with $\alpha > 1$ is more challenging. This is not surprising, as $\alpha > 1$ tends to generate more uniform distributions, which are not informative of the causal relationship between nodes.

In the second set of experiments, we compared CSIvA to non-linear ICP and DAG-GNN. To limit the number of experiments to run, we set $\alpha = 1.0$, as this gives the least amount of prior information to CSIvA. As shown in Figure 4, CSIvA significantly outperforms non-linear ICP and DAG-GNN. CSIvA achieves $\mathcal{H} < 5$ on size 10 graphs, almost half of the error rate compared to non-linear ICP and DAG-GNN, both achieving a significantly higher Hamming distance ($\mathcal{H} = 9.3$ and $\mathcal{H} = 9.5$ respectively) on larger and denser graphs.

Amount of samples. We evaluated CSIvA on different amount of samples $(100, 200, 500, 1000, 1500)$ per CBNs. Results for Dirichlet data sampled from $N = 10$ graphs are shown in Figure 5. We can see that 1000 samples are sufficient for ER-1 graphs, whereas having 1500 samples gives slightly better results compared to 1000 samples for ER-2 graphs.

6.2 Out-of-distribution experiments

In this set of experiments, we evaluated CSIvA's ability to generalize to aspects of the data generating distribution that are often unknown, namely graph density and parameters of the CPDs, such as the α values of the Dirichlet distribution. Hence, these experiments investigate how well CSIvA generalizes when graph sparsity and alpha values for the Dirichlet distribution of the training data differ from the test data.

Varying graph density. We evaluate how well CSIvA performs when trained and tested on CBNs with varying graph density on MLP and $\alpha = 1$ Dirichlet data. We fixed the number of nodes to $N = 7$, with variables able to take on discrete values in $\{1, 2, 3\}$. The graphs in training and test datasets can take ER degree $\in \{1, 2, 3\}$. Results are shown in Table 1 for the MLP data and Table 2 for the Dirichlet data. For the MLP data, models trained on ER-2 graph generalizes the best. For

[2] Without this modification, the method achieved near chance performance.

Train		ER-1	ER-2	ER-3
Test	ER-1	1.2	0.9	1.3
	ER-2	3.3	1.8	2.1
	ER-3	5.0	2.8	2.8

Table 1: **Results on varying graph density for MLP data:** Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices.

Train		ER-1	ER-2	ER-3
Test	ER-1	0.19	0.21	0.28
	ER-2	0.86	0.29	0.25
	ER-3	1.61	0.60	0.23

Table 2: **Results on generalization on graph sparsity for Dirichlet data ($\alpha = 1$):** Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices.

Dirichlet data, there isn't one value of graph density that consistently generalizes best across graphs with different densities. Nevertheless, ER-2 graphs give a balanced trade-off and generalizes well across graphs with different sparsity.

Varying α. We evaluate CSIvA on training and test data coming from Dirichlet distributions with $\alpha \in \{0.1, 0.25, 0.5\}$. Results for ER-1 graphs with $N = 7$ are found in Table 3. There isn't a value of α that performs consistently well across different values of α for the test data. Nevertheless, $\alpha = 0.25$ is a balanced trade-off and generalizes well across test data with $0.1 \leq \alpha \leq 0.5$.

Train		$\alpha = 0.1$	$\alpha = 0.25$	$\alpha = 0.5$
Test	$\alpha = 0.1$	0.31	0.33	0.52
	$\alpha = 0.25$	0.72	0.40	0.41
	$\alpha = 0.5$	1.8	0.71	0.35

Table 3: **Results on varying graph density for Dirichlet data:** Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices.

6.3 Sim-to-real experiments

In this final set of experiments, we evaluated CSIvA's ability to generalize from being trained on MLP and Dirichlet data to being evaluated on the widely used Sachs (Sachs et al., 2005) and Asia (Lauritzen & Spiegelhalter, 1988) CBNs from the BnLearn repository, which have $N = 11$ and $N = 8$ nodes respectively. We followed the established protocol from Ke et al. (2020a); Lippe et al. (2021); Scherrer et al. (2021) where we sampled observational and interventional data from the CBNs provided by the repository. These experiments are the most important test of our hypothesis that causal structure of synthetic datasets can be a useful proxy for discovering causal structure in realistic settings.

We emphasize that all hyperparameters for the MLP and Dirichlet data generation and for the learning procedure were chosen without using the Sachs and Asia data; only after the architecture and parameters were finalized was the model tested on these benchmarks. Furthermore, to keep the setup simple, we trained on data sampled from a single set of hyperparameters instead of a broader mixture. Findings in Section 6.2 suggest that ER-2 graphs with $\alpha = 0.25$ generalize well overall and hence were chosen.

We report the results in Table 4. We compare to a range of baselines from Heinze-Deml et al. (2018a); Yu et al. (2019); Gamella & Heinze-Deml (2020) and others. Note that we do not compare to the

	Sachs	Asia
All-absent Baseline	17	8
GES Chickering (2002)	19	4
DAG-notears Zheng et al. (2018)	22	14
DAG-GNN Yu et al. (2019)	13	8
GES Hauser & Bühlmann (2012)	16	11
ICP Peters et al. (2016)	17	8
Non-linear ICP Heinze-Deml et al. (2018b)	17	7
CSIvA (MLP data)	**6**	**3**
CSIvA (Dirichlet data)	**5**	**3**

Table 4: **Results on Sachs and Asia data:** Hamming distance $\mathcal{H}$ between predicted and ground-truth adjacency matrices.

method in Ke et al. (2020a), as this method needs at least $500,000$ data samples (which is more than 300 times the amount required by CSIvA).

CSIvA trained on both the MLP data and on the Dirichlet data significantly outperforms all other methods on both the Asia and the Sachs dataset. This serves as strong evidence that CSIvA can learn to induce causal structures in the more realistic real-world CBNs, while only trained on synthetic data.

7 Discussion

In this paper, we have presented a novel approach towards causal graph structure inference. CSIvA is based on learning from synthetic data in order to obtain a strong learning signal (in the form of explicit supervision), using a novel transformer-based architecture which directly analyzes the data and computes a distribution of candidate graphs. We demonstrated that even though only trained on synthetic data, CSIvA generalizes on out-of-distribution.

We see several possible extensions to CSIvA. The distribution of the synthetic data used for training determines the inductive bias of the trained network. Identifying which priors lead to the best performance in real-world scenarios and how to convert informal prior knowledge into better priors would potentially improve robustness of our solution. Another venue of improvement would be to combine supervised learning on synthetic data with score optimization. Note that since CSIvA offers a probabilistic distribution of possible graphs, it is in principle possible to train it by reinforcement learning (RL) methods such as REINFORCE (Williams, 1992) on any score function that can be computed on a graph.

An even more intriguing alternative is to leverage the output distribution of a trained network as a guide for a search-based method which optimizes a well designed score function. This would in particular enable CSIvA to become less black-box, as the trained network would only be used to generate proposals for plausible causal graphs, which can then be evaluated by and chosen on the basis of more interpretable metrics.

On the computational side of things, CSIvA is based on transformers, which uses self-attention. Standard transformer implementation that uses self-attention scales quadratically with the length of the inputs. This makes it challenging for CSIvA to scale to larger graphs. However, methods such as Jaegle et al. (2021); Goyal et al. (2021b) enable transformers to scale linearly with the number of inputs (and outputs), which can be readily incorporated into our framework. Further work is required to scale our method to very large datasets.

Finally, another possible direction of future work would be to use the proposed framework for learning causal structure from raw visual data. This could be useful, e.g., in an RL setting in which an RL agent interacts with the environment via observing low level pixel data. Such an agent would need to infer the causal variables underlying the observations, as well as their relationships (Ahmed et al., 2020; Ke et al., 2021; Wang et al., 2021).

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A Transformer Neural Networks

The transformer architecture, introduced in Vaswani et al. (2017), is a multi-layer neural network architecture using stacked self-attention and point-wise, fully connected, layers. The classic transformer architecture has an encoder and a decoder, but the encoder and decoder do not necessarily have to be used together.

Scaled dot-product attention. The attention mechanism lies at the core of the transformer architecture. The transformer architecture uses a special form of attention, called the scaled dot-product attention. The attention mechanism allows the model to flexibility learn to weigh the inputs depending on the context. The input to the QKV attention consists of a set of queries, keys and value vectors. The queries and keys have the same dimensionality of d_k, and values often have a different dimensionality of d_v. Transformers compute the dot products of the query with all keys, divide each by $\sqrt{d_k}$, and apply a softmax function to obtain the weights on the values. In practice, transformers compute the attention function on a set of queries simultaneously, packed together into a matrix Q. The keys and values are also packed together into matrices K and V. The matrix of outputs is computed as: $\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d_k}})V$.

Encoder. The encoder is responsible for processing and summarizing the information in the inputs. The encoder is composed of a stack of N identical layers, where each layer has two sub-layers. The first sub-layer consists of a multi-head self-attention mechanism, and the second is a simple, position-wise fully connected feed-forward network. Transformers employ a residual connection (He et al., 2016) around each of the two sub-layers, followed by layer normalization Ba et al. (2016). That is, the output of each sub-layer is $\text{LayerNorm}(x + \text{Sublayer}(x))$, where $\text{Sublayer}(x)$ is the function implemented by the sub-layer itself.

Decoder. The decoder is responsible for transforming the information summarized by the encoder into the outputs. The decoder also composes of a stack of N identical layers, with a small difference in the decoder transformer layer. In addition to the two sub-layers in each encoder layer, a decoder layer consists of a third sub-layer. The third sub-layer performs a multi-head attention over the output of the encoder stack. Similar to the encoder, transformers employ residual connections around each of the sub-layers, followed by layer normalization. Transformers also modify the self-attention sub-layer in the decoder stack to prevent positions from attending to subsequent positions. This masking, combined with fact that the output embeddings are offset by one position, ensures that the predictions for position i can depend only on the known outputs at positions less than i.

B Detailed results.

Detailed results for experiments in Section 6.1 and 6.2 are described in the tables below.

B.1 Results on continuous data

Results for comparions between the proposed model CSIvA and baselines non-linear ICP (Yu et al., 2019) and DAG-GNN (Heinze-Deml et al., 2018a) are shown in Table 5. Both non-linear ICP and the proposed model CSIvAperforms well on the data. DAG-GNN (Yu et al., 2019), both are significantly better compared to DAG-GNN, which only takes observational data.

B.2 Results on MLP data

Results for comparisons between CSIvA and baselines non-linear ICP (Yu et al., 2019) and DAG-GNN (Heinze-Deml et al., 2018a) on MLP data are shown in Table 6. MLP data is non-linear and hence more challenging compared to the continuous linear data. CSIvA significantly outperforms non-linear ICP and DAG-GNN. The difference becomes more apparent as the graph size grows larger and more dense.

	ER = 1			ER = 2		
	Var = 5	**Var = 7**	**Var = 10**	**Var = 5**	**Var = 7**	**Var = 10**
All-absent Model	2.50	3.50	5.00	5.00	7.00	10.00
Yu et al. (2019)	2.71	3.62	4.76	5.20	8.81	13.00
Heinze-Deml et al. (2018b)	0.47	0.61	1.10	0.90	1.40	2.41
CSIvA	**0.12**	**0.20**	**0.35**	**0.81**	**1.22**	**1.73**

Table 5: **Results on Continuous data**. Hamming distance $\mathcal{H}$ for learned and ground-truth edges on synthetic graphs, compared to other methods, averaged over 128 sampled graphs. The number of variables varies from 5 to 10, expected degree = 1 or 2, and the value of variables are drawn from $\mathcal{N}(0, 0.1)$. Note that for (Heinze-Deml et al., 2018a), the method required nodes to be causally ordered, and 20 repeated samples taken per intervention, as interventions were continuously valued. "All-absent model" is a model that outputs an empty adjacency matrix.

	ER = 1			ER = 2		
	Var = 5	**Var = 7**	**Var = 10**	**Var = 5**	**Var = 7**	**Var = 10**
All-absent Model	2.50	3.50	5.00	5.00	7.00	10.00
Yu et al. (2019)	2.52	4.61	7.30	4.33	6.51	12.78
Heinze-Deml et al. (2018b)	2.43	3.27	4.62	4.76	6.61	9.12
CSIvA	**0.98** $\pm$ 0.16	**1.83** $\pm$ 0.84	**2.25** $\pm$ 0.17	**1.51** $\pm$ 0.47	**3.41** $\pm$ 0.48	**5.12** $\pm$ 0.26

Table 6: **Results on MLP data**. Hamming distance $\mathcal{H}$ for learned and ground-truth edges on synthetic graphs, compared to other methods, averaged over 128 sampled graphs ($\pm$ standard deviation). The number of variables varies from 5 to 10, expected degree = 1 or 2, and the dimensionality of the variables are fixed to 3. We compared to the strongest baseline model that uses observational data (Yu et al., 2019) and also the strongest that uses interventional data (Heinze-Deml et al., 2018a). Note that for (Heinze-Deml et al., 2018a), the method required nodes to be causally ordered, and Gaussian noise $\mathcal{N}(0, 0.1)$ to be added. "All-absent model" is an baseline model that outputs all zero edges for the adjacency matrix.

B.3 Results on Dirichlet data.

Results for comparisons between our model CSIvA and baselines non-linear ICP (Yu et al., 2019) and DAG-GNN (Heinze-Deml et al., 2018a) on Dirichlet data are shown in Table 7. MLP data is non-linear and hence more challenging compared to the continuous linear data. Our model CSIvAsignificantly outperforms non-linear ICP and DAG-GNN. The difference becomes more apparent as the graph size grows larger and more dense. We also compare how different alpha values of Dirichlet data impacts

	ER = 1			ER = 2		
	Var = 5	**Var = 7**	**Var = 10**	**Var = 5**	**Var = 7**	**Var = 10**
All-absent Model	2.5	3.5	5.0	5.0	7.0	10.0
(Yu et al., 2019)	1.75	4.5	4.0	4.5	7.25	9.50
(Heinze-Deml et al., 2018a)	2.2	3.2	5.3	4.7	6.1	9.3
CSIvA	**0.26** $\pm$ 0.05	**0.83** $\pm$ 0.06	**2.37** $\pm$ 0.07	**0.65** $\pm$ 0.05	**0.97** $\pm$ 0.06	**4.59** $\pm$ 0.08

Table 7: **Results on Dirichlet data.** Hamming distance $\mathcal{H}$ for learned and ground-truth edges on synthetic graphs, compared to other methods, averaged over 128 sampled graphs ($\pm$ standard deviation). The number of variables varies from 5 to 10, expected degree = 1 or 2, the dimensionality of the variables are fixed to 3, and the α is fixed to 1.0. We compare to the strongest causal-induction methods that uses observational data (Yu et al., 2019) and the strongest that uses interventional data (Heinze-Deml et al., 2018a).

learning for our model. CSIvA performs well on all graphs where $\alpha \leq 0.5$, and the performance starts to degard as $alpha = 1.0$. When $\alpha = 5.0$, CSIvAis almost performing similarly to the

All-absent model (outputting all zero edges). This is to be expected, as larger alpha values is less informative of the causal relationships between variables.

	ER = 1			**ER = 2**		
	Var = 5	**Var = 7**	**Var = 10**	**Var = 5**	**Var = 7**	**Var = 10**
$\alpha = 0.1$	0.18	0.37	0.72	0.39	0.84	1.27
$\alpha = 0.25$	0.14	0.41	0.77	0.29	0.64	1.27
$\alpha = 0.5$	0.14	0.43	0.94	0.41	0.79	2.11
$\alpha = 1.0$	0.27	0.63	2.31	0.68	1.22	4.32
$\alpha = 5.0$	1.27	2.56	4.91	3.21	7.0	9.99
All-absent Model	2.5	3.5	5.0	5.0	7.0	10.0

Table 8: **Results on Dirichlet data.** Hamming distance $\mathcal{H}$ (lower is better) for learned and ground-truth edges on synthetic graphs, averaged over 128 sampled graphs. The proposed model accomplished a hamming distance of less than 2.5 for Dirichlet data with $\alpha <= 0.5$.