Learning semi-Markovian DAGs with flow-based VAE

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December 11, 2023

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Overview

- **Problem**: Learning semi-Markovian DAGs
- **Solution**: Normalizing flow based VAE
- **Contribution**
  - A new method for learning semi-Markovian DAGs
  - A new method for learning DAGs with non-Gaussian noise

DAG and SEM

- Directed Acyclic Graph(DAG) $\mathcal{G} = (V, E)$ with $V = \{1, \ldots, m\}$ is used to represent a causal structure[1]
- Linear Structural Equation Model(SEM) is defined as

$$X_i = \sum_{j \in \mathrm{Pa}(i)} \beta_{ij} X_j + \epsilon_i$$

  where ϵ_i is a noise variable.
- Matrix form can be written as

$$\mathbf{X} = \mathbf{A}^T \mathbf{X} + \epsilon \tag{1}$$

  where $\mathbf{A}$ is an adjacency matrix of $\mathcal{G}$ and ϵ is a noise vector.

[1] Pearl, *Causality*.

DAG and SEM(Cont'd)

- If $(\mathbf{I}-\mathbf{A}^T)$ is nonsingular, SEM can be written as

$$\mathbf{X} = (\mathbf{I}-\mathbf{A}^T)^{-1}\epsilon \tag{2}$$

- Usually we assume $\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{\Sigma})$ and

$$\mathbf{X} \sim \mathcal{N}(\mathbf{0}, (\mathbf{I}-\mathbf{A}^T)^{-1}\mathbf{\Sigma}(\mathbf{I}-\mathbf{A})^{-1})$$

Semi-Markovian DAG

- Semi-Markovian DAG is a DAG where the noise variables have dependencies[2]
- The noise vector ϵ is a semi-Markovian noise vector if

$$\Sigma \in \mathcal{W}(G) := \{\Sigma \in \mathbb{R}^{m \times m} : \Sigma_{ij} = \Sigma_{ji} = 0 \text{ if } i \notin \text{sib}(j)\} \quad (3)$$

where $\text{sib}(j) = \{i : i \sim j \text{ in } G\}$[3]

- Learn cyclic adjacency matrix or acyclic adjacency matrix

[2] Shpitser and Pearl, "Identification of Joint Interventional Distributions in Recursive Semi-Markovian Causal Models".

[3] Wang and Drton, "Empirical likelihood for linear structural equation models with dependent errors".

DAG Learning

- DAG learning is a problem of estimating $\mathcal{G}$ from $\mathbf{X}$
- NP-hard problem[4]
- Score-based methods[5] and constraint-based methods[6] are used
- NOTEARS[7]: Combinatorial optimization to Continuous optimization problem

$$\min_{\mathbf{A}} F(A) \text{ subject to } G(A) \in \mathbb{D} \Rightarrow \min_{\mathbf{A}} F(A) \text{ subject to } h(A) = 0$$

where $\mathbb{D}$ denotes the discrete space of DAGs on m nodes and $h(A) = 0$ iff $G(A)$ is acyclic.

[4] Chickering, Meek, and Heckerman, "Large-Sample Learning of Bayesian Networks is NP-Hard".
[5] Spirtes, Glymour, and Scheines, *Causation, Prediction, and Search*.
[6] Chickering, "Optimal Structure Identification with Greedy Search".
[7] Zheng et al., *DAGs with NO TEARS: Continuous Optimization for Structure Learning*.

DAG Learning(Cont'd)

Theorem

A matrix $\mathbf{A}$ is the adjacency matrix of a DAG if and only if

$$h(A) = \mathrm{tr}(\exp(\mathbf{A} \circ \mathbf{A})) = \mathrm{m}$$

where $\circ$ denotes the Hadamard product.

Theorem

A matrix $\mathbf{A}$ is the adjacency matrix of a DAG if and only if

$$\mathrm{tr}[(\mathrm{I} + \alpha\mathbf{A} \circ \mathbf{A})^{\mathrm{m}}] = \mathrm{m}$$

for any $\alpha > 0$.

VAE

- Variational Autoencoder(VAE) is a generative model that learns a latent variable model
- It is trained by maximizing the evidence lower bound(ELBO)

$$\mathcal{L}(\theta, \phi; \mathbf{x}) = \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathrm{KL}(q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})) \tag{4}$$

- $q_\phi(\mathbf{z}|\mathbf{x})$ is an approximate posterior and $p_\theta(\mathbf{x}|\mathbf{z})$ is a generative model

Normalizing Flow

- Normalizing flow transforms a simple distribution to a complex distribution[8]
- It is a sequence of invertible transformations $f_t : \mathbb{R}^d \to \mathbb{R}^d$

$$z_T = f_T \circ f_{T-1} \circ \cdots \circ f_1(z_0) \tag{5}$$

- The probability density function of z_T is

$$p(z_T) = p(z_0) \left| \det \left(\frac{\partial f_T \circ f_{T-1} \circ \cdots \circ f_1(z_0)}{\partial z_0} \right) \right| \tag{6}$$

[8] Rezende and Mohamed, "Variational Inference with Normalizing Flows".

Linear IAF

- Inverse Autoregressive Flow(IAF) is a normalizing flow that uses autoregressive transformation[9]
- Linear IAF is a special case of IAF where f_t is a linear transformation

$$\mathbf{z_t} = \mu_\mathbf{t} + \sigma_\mathbf{t} \odot \mathbf{z_{t-1}}. \tag{7}$$

- Transformation of the linear IAF can be written as

$$\mathbf{z}_T = \mathbf{L}(\mathbf{x}) \cdot \mathbf{z}_0. \tag{8}$$

where $\mathbf{L}(\mathbf{x})$ is a lower triangular matrix from encoder network.
- We can use more flexible prior distribution by using normalizing flow.
- When $\mathbf{z}_0$ has diagonal covariance, $\mathbf{z}_T$ then has full covariance matrix.

[9] Kingma et al., "Improved Variational Inference with Inverse Autoregressive Flow".

Model

Overall architecture of our model is shown in Figure below.

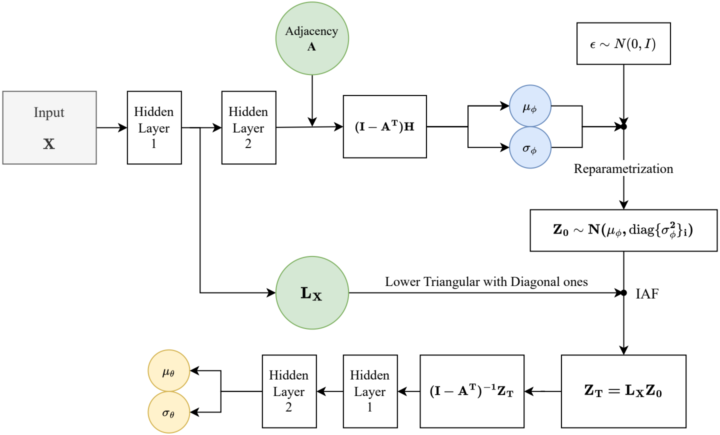

Figure: Overall architecture of our model

Learning

- The optimization procedure is minimizing the following loss function:

$$\mathcal{L}(A, W, \lambda) = -\mathcal{L}_{\mathrm{ELBO}} + \tau \|A\|_1 + \lambda h(A) + \frac{c}{2}|h(A)|^2. \tag{9}$$

- The second term is the L1 regularization term, which encourages sparsity of the adjacency matrix.
- $\tau = 0.1 \times (\frac{m}{50})^2$ works well in our experiment setting.
- The third and fourth terms are the augmented Lagrangian terms.
- Gradually increasing the value of c during the training process results the acyclicity constraint to zero.

Experiment

- We compare our method with the DAG-GNN[10] with random graph datasets.
- thresholding value of extracting graph as 0.3
- Erdős–Rényi random graph with 5000 samples
- Node size : 10, 20, 30, and 50 nodes
- Noise type : (Independent) Gaussian, Laplace, Exponential and (Dependent) Gaussian

[10] Yu et al., "DAG-GNN: DAG Structure Learning with Graph Neural Networks".

Experiment(Cont'd)

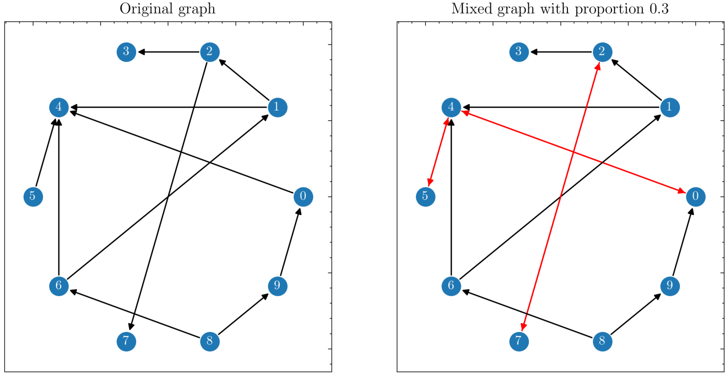

Figure: Example of mixed graph

Experiment(Cont'd)

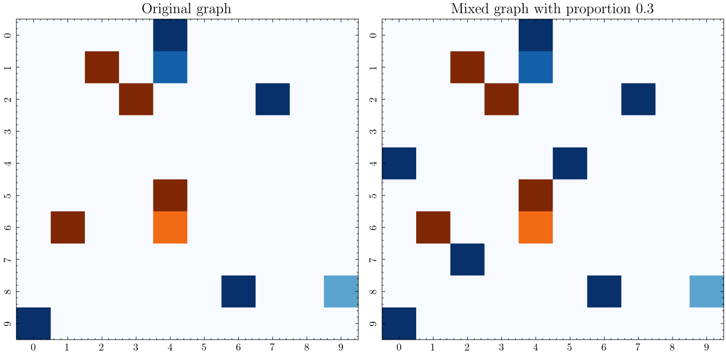

Figure: Adjacency matrix of previous example graph

Experiment(Cont'd)

- We evaluate the performance of our method using two metrics: Structural Hamming Distance (SHD), False Discovery Rate (FDR) with respect to the number of predicted edges.
- SHD measures the number of edge additions, deletions, and reversals required to transform the estimated graph into the true graph.
- FDR represents the ratio of false positives to the total number of predicted edges.
- These metrics are calculated by comparing the estimated graph with the true DAG.
- For each combination, we generate at least 5 random graphs and calculate the average metrics.

Independent Noise

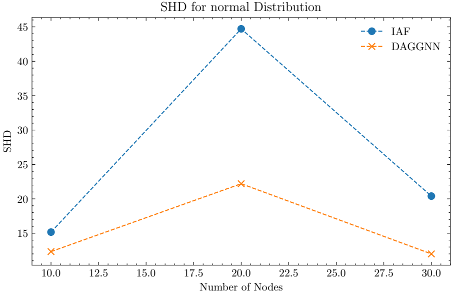

Figure: SHD with normal

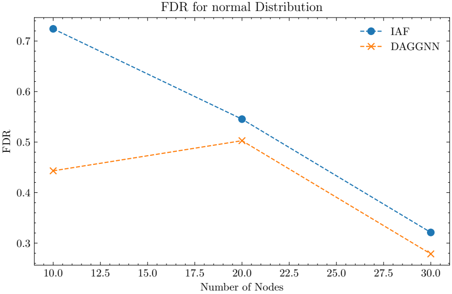

Figure: FDR with normal

- In the case of independent Gaussian noise, DAG-GNN(orange) performs better than our method(blue).

Independent Noise(Cont'd)

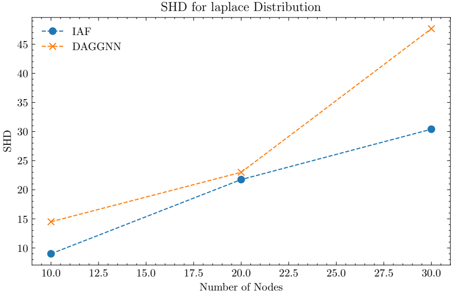

Figure: SHD with Laplace

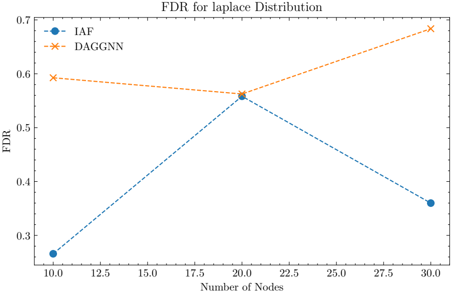

Figure: FDR with Laplace

In the case of independent Laplace noise, our method(blue) performs better than DAG-GNN(orange).

Independent Noise(Cont'd)

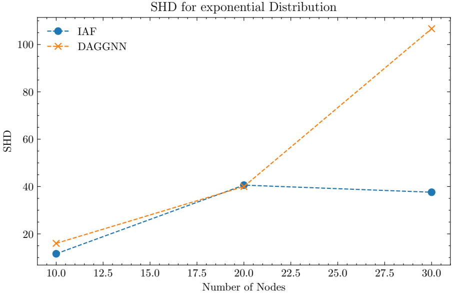

Figure: SHD with Exponential

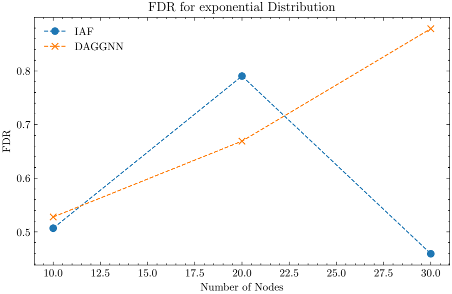

Figure: FDR with Exponential

In the case of independent Exponential noise, our method(blue) performs better than DAG-GNN(orange).

Independent Noise(Cont'd)

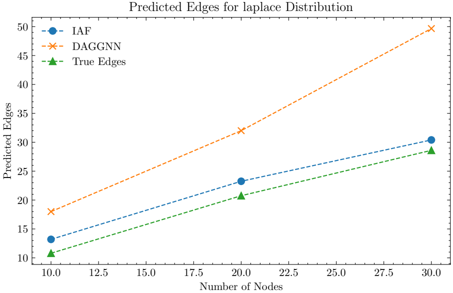

Figure: Number of predicted edges with Laplace

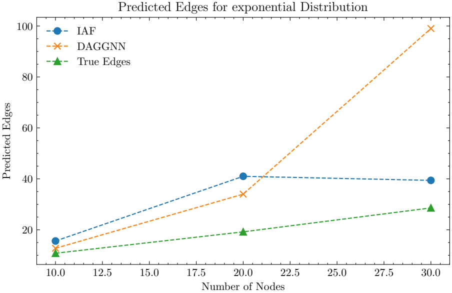

Figure: Number of predicted edges with Exponential

Considering the number of predicted edges with the SHD and FDR, our method(blue) performs better than DAG-GNN(orange).

Figure: Comparison of estimated graphs with Laplace(above) and Exponential(below) noise

Dependent Noise

Proportion of bidirectional edges fixed to 0.3.

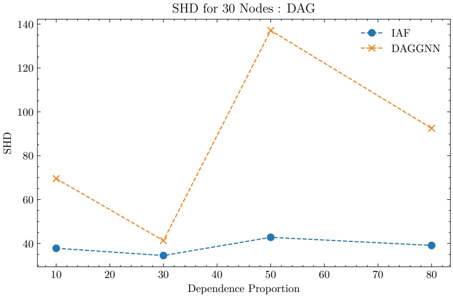

Figure: SHD with dependent Gaussian

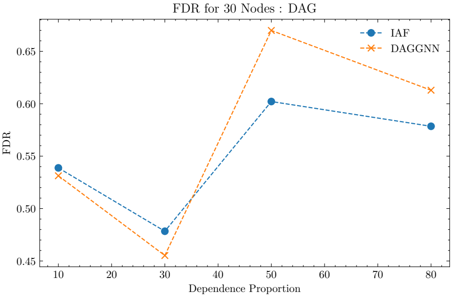

Figure: FDR with dependent Gaussian

Dependent Noise(Cont'd)

Proportion of bidirectional edges fixed to 0.3.

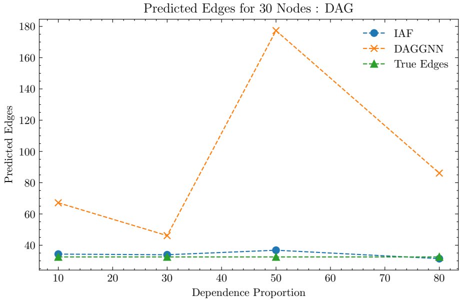

Figure: Number of predicted edges with dependent Gaussian

- In the case of dependent Gaussian noise, our method(blue) performs better than DAG-GNN(orange).
- Considering the stable number of predicted edges with the SHD and FDR, our method(blue) outperforms.

Dependent Noise(Cont'd)

Node size $m = 10$: similar performance between DAG-GNN(orange) and our method(blue).

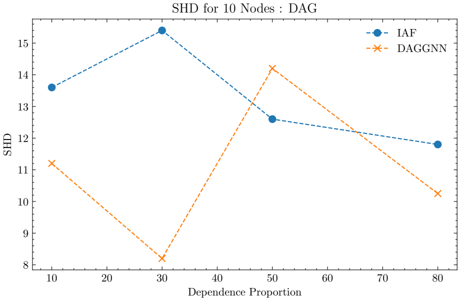

Figure: SHD with dependent Gaussian

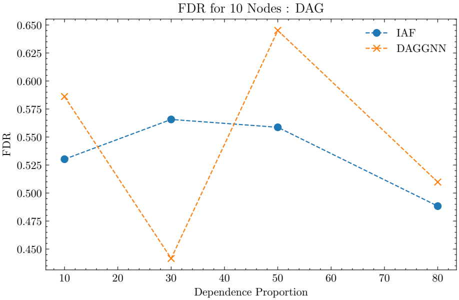

Figure: FDR with dependent Gaussian

Dependent Noise(Cont'd)

Node size $m = 20$: our method(blue) performs better than DAG-GNN(orange).

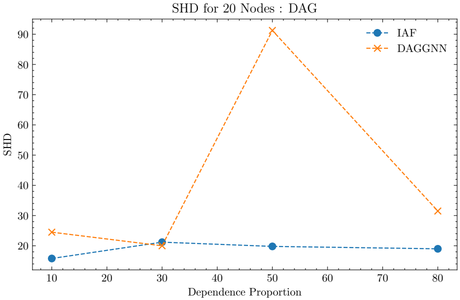

Figure: SHD with dependent Gaussian

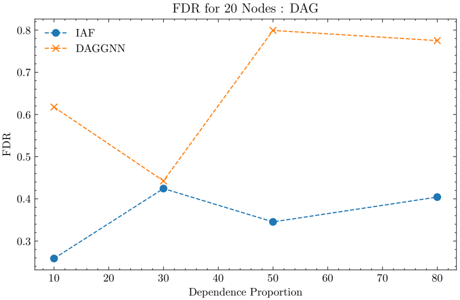

Figure: FDR with dependent Gaussian

Dependent Noise(Cont'd)

Node size $m = 30$: our method(blue) performs better than DAG-GNN(orange).

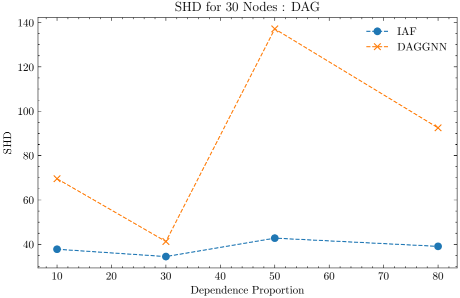

Figure: SHD with dependent Gaussian

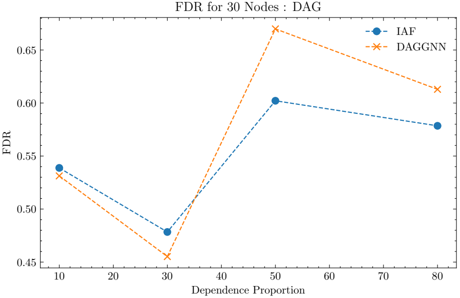

Figure: FDR with dependent Gaussian

Dependent Noise(Cont'd)

Node size $m = 50$: our method(blue) performs better than DAG-GNN(orange).

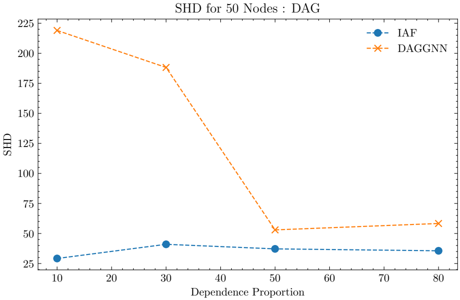

Figure: SHD with dependent Gaussian

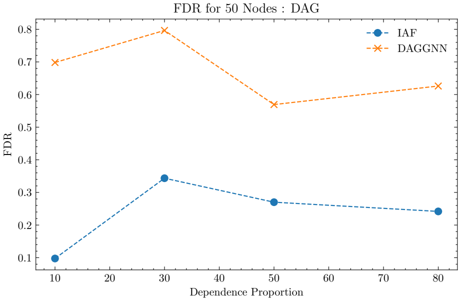

Figure: FDR with dependent Gaussian

Number of predicted edges

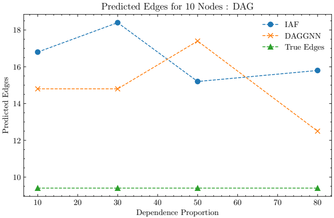

Figure: $m = 10$

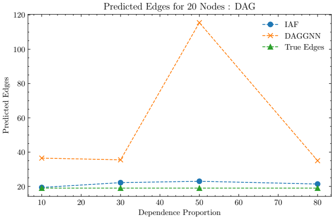

Figure: $m = 20$

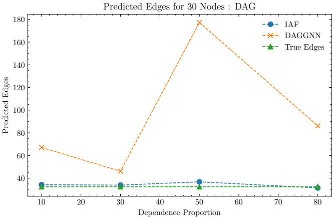

Figure: $m = 30$

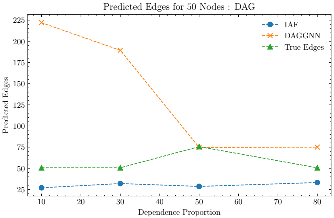

Figure: $m = 50$

Conclusion

- Proposed a method to learn the structure of a semi-Markovian DAG using a flow-based VAE.
- Conducted experiments on simulated data and compared the performance of our method with that of DAG-GNN.
- Our method outperforms DAG-GNN in terms of both SHD and FDR metrics, especially when the noise variables have a dependent structure and when the size of the graph is large.
- In terms of the number of predicted edges, our method results in fewer edges than DAG-GNN while maintaining the same or better level of SHD and FDR.

Conclusion(Cont'd)

- However, contrary to our initial expectations, the lower triangular matrix $\mathbf{L}$ learned in the IAF layer did not capture the covariance matrix of the actual noise variables.
- This seems to be due to the entanglement problem in the latent space, and resolving this issue remains a future research task.
- If the full covariance matrix of the noise variables could be found, it could be possible to directly identify bidirectional edges in the graph, enabling more accurate learning of the semi-Markovian graph.

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