Learning semi-Markovian DAGs with flow-based VAE

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December 12, 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 [4]
- 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

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

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

DAG and SEM (cont'd)

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

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

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

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

- In most cases, we assume $\mathbf{\Sigma} = \mathbf{I}$ or $\mathbf{\Sigma} = \mathbf{D}$ where $\mathbf{D}$ is a diagonal matrix.
- DAG-GNN [9] generalizes linear SEM using a deep neural network.

$$f_2^{-1}(X) = A^T f_2^{-1}(X) + f_1(Z),$$

Semi-Markovian DAG

- DAGs have many convenient properties (e.g. Markov property, d-separation, etc.)
- More general class of DAGs is acyclic directed mixed graphs (ADMGs) i.e. semi-Markovian DAGs
- Semi-Markovian DAG is a DAG where the noise variables have dependencies [6]
- The noise vector ϵ is a semi-Markovian noise vector if

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

  where $\text{sib}(j) = \{i : i \sim j \text{ in } G\}$ [8]
- Learn cyclic adjacency matrix [8] or acyclic adjacency matrix

DAG Learning

- DAG learning is a problem of estimating $\mathcal{G}$ from $\mathbf{X}$
- NP-hard problem [2]
- Score-based methods [7] and constraint-based methods [1] are used
- NOTEARS[10]: 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.

DAG Learning (cont'd)

Theorem

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

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

where $\circ$ denotes the Hadamard product.

Theorem

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

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

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)

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

- $q_\phi(\mathbf{z}|\mathbf{x})$ 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 [5]
- It is a sequence of invertible transformations $f_t : \mathbb{R}^d \to \mathbb{R}^d$

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

- The probability density function of z_T is

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

Linear IAF

- Inverse Autoregressive Flow(IAF) is a normalizing flow that uses autoregressive transformation [3]

$$\mathbf{z}_0 = \mu_0 + \sigma_0 \odot \epsilon, \quad \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$$
$$\mathbf{z}_t = \mu_t + \sigma_t \odot \mathbf{z}_{t-1}.$$

- Linear IAF is the simplest case of IAF where f_t is a linear transformation
- Transformation of the linear IAF can be written as

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

where $\mathbf{L}(\mathbf{x})$ is a lower triangular matrix from encoder network.

Linear IAF (cont'd)

- $\mathbf{L}$ can be regarded as a cholesky decomposition of covariance matrix.
- 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.
- The KL divergence term of ELBO can be written as

$$\begin{aligned} D_{KL}(q_\phi(\mathbf{z}_0|\mathbf{x})\|p(\mathbf{z}_T)) &= \log q_\phi(\mathbf{z}_0|\mathbf{x}) - \log p(\mathbf{z}_T) \\ &= -\frac{1}{2}(\mathbf{z}_0 - \mu_\phi)^T \Sigma_\phi^{-1}(\mathbf{z}_0 - \mu_\phi) + \frac{1}{2}\mathbf{z}_T^T \mathbf{z}_T \end{aligned}$$

where μ_ϕ and Σ_ϕ are the mean and covariance matrix from the encoder network.

Model

Overall architecture of our model is shown in Figure below.

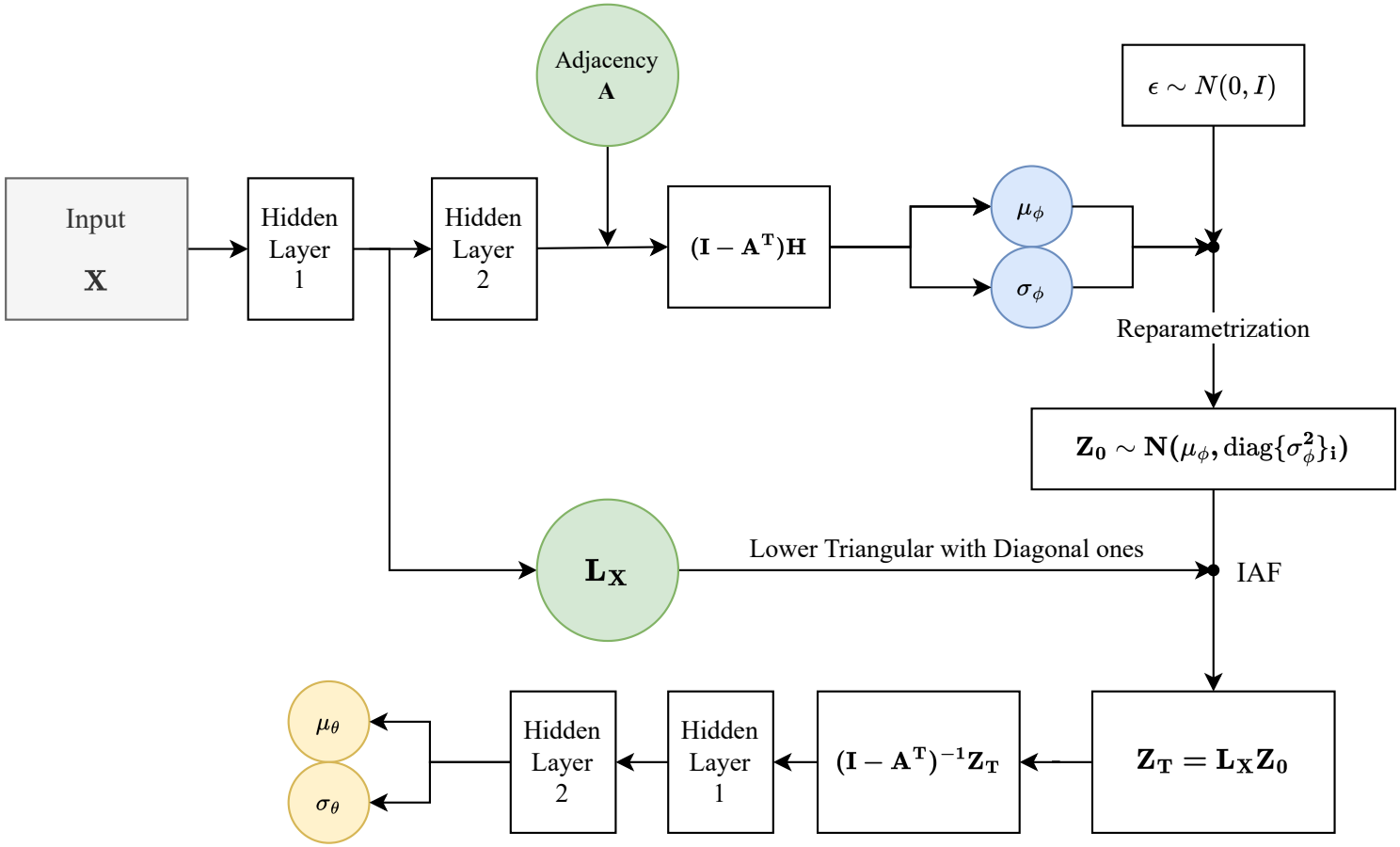

Figure: Overall architecture of our model

Learning

- The optimization procedure is minimizing the following loss function:

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

- 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 [9] 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 : $\epsilon_i \sim \mathcal{N}(0, 1)$, $\epsilon_i \sim \text{Laplace}(0, 1)$, $\epsilon_i \sim \text{Exp}(1)$
  - Dependent : $\epsilon_i \sim \mathcal{N}(0, \mathbf{\Sigma})$ where $\mathbf{\Sigma}$ is a covariance matrix of semi-Markovian DAG

Experiment (cont'd)

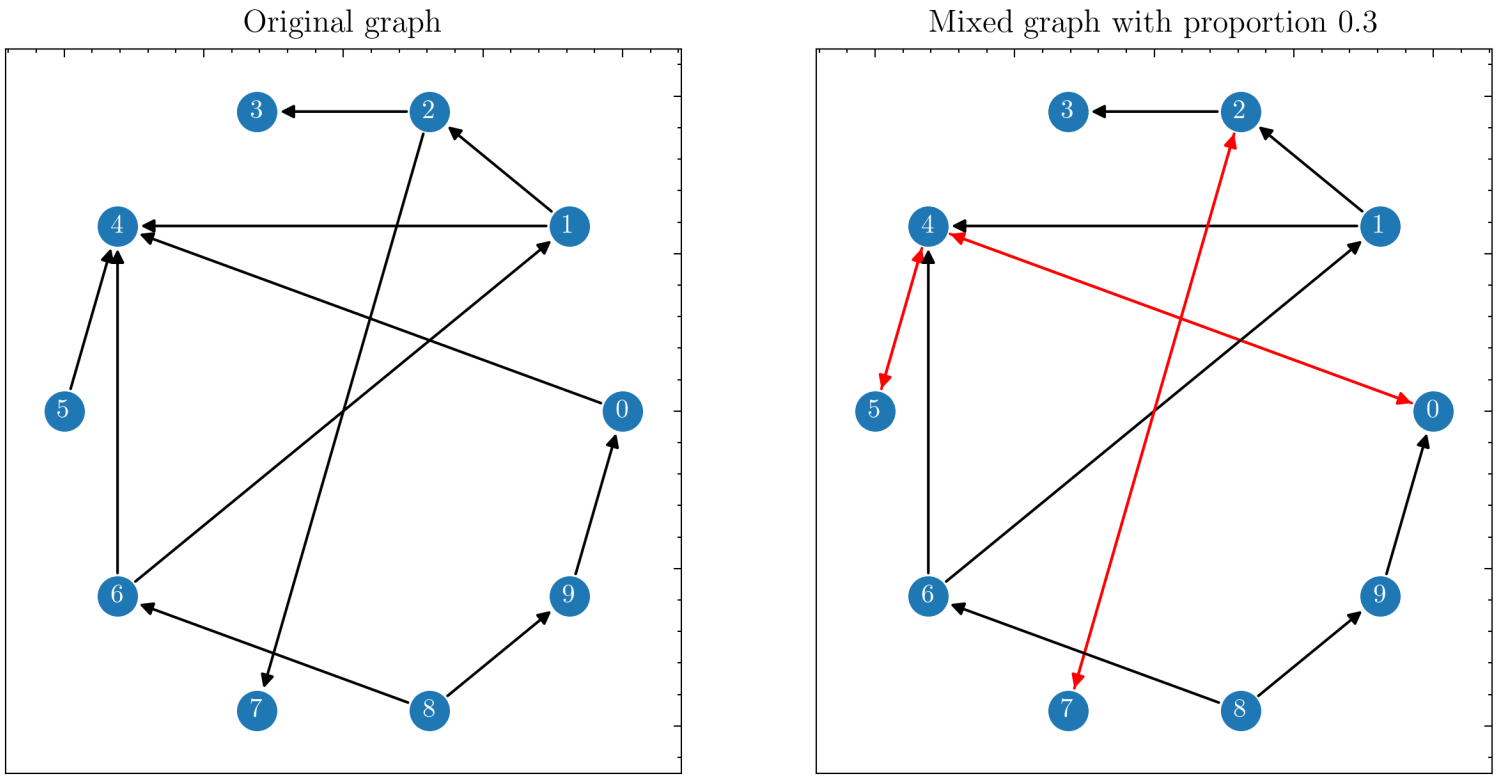

Figure: Example of mixed graph

Experiment (cont'd)

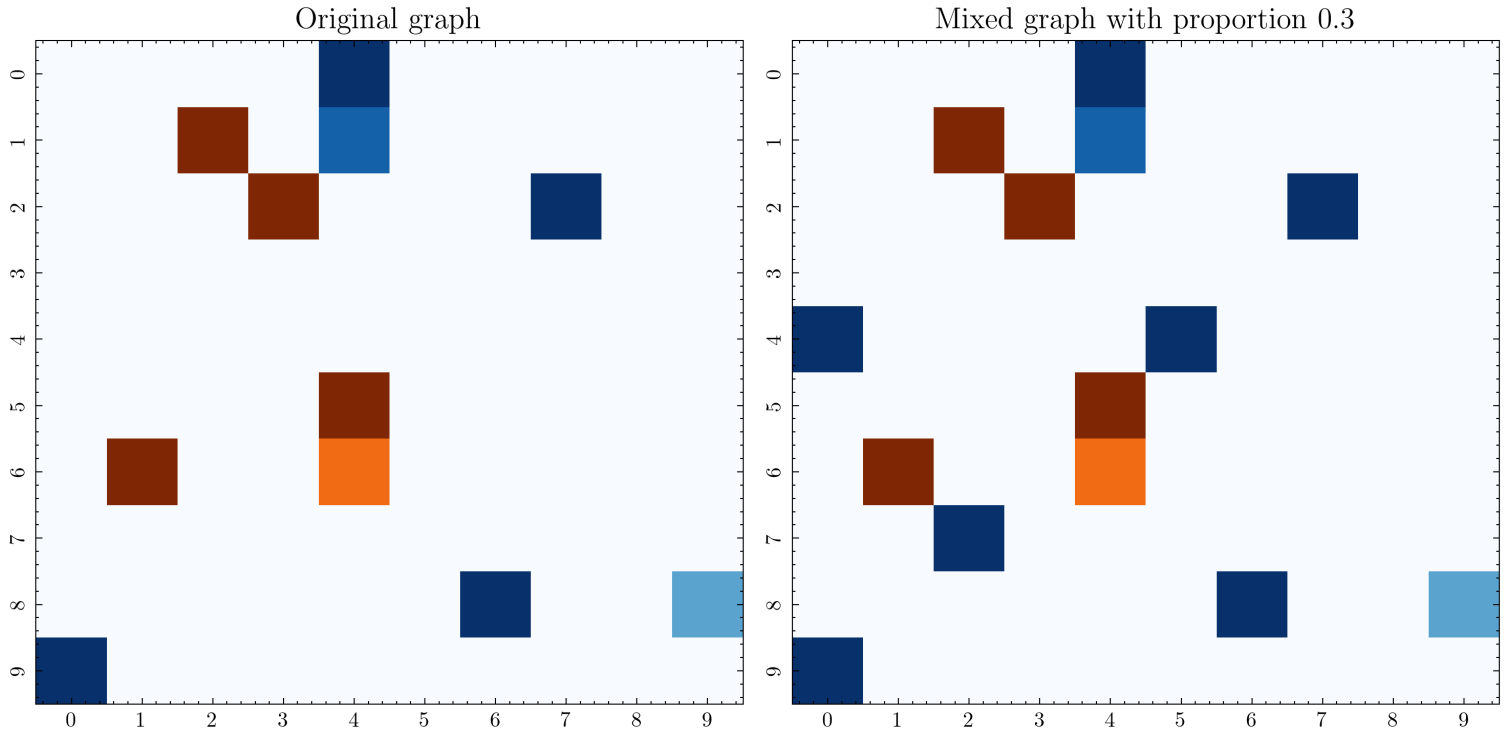

Figure: Adjacency matrix of previous example graph

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 measures the proportion of incorrectly predicted edges among the 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

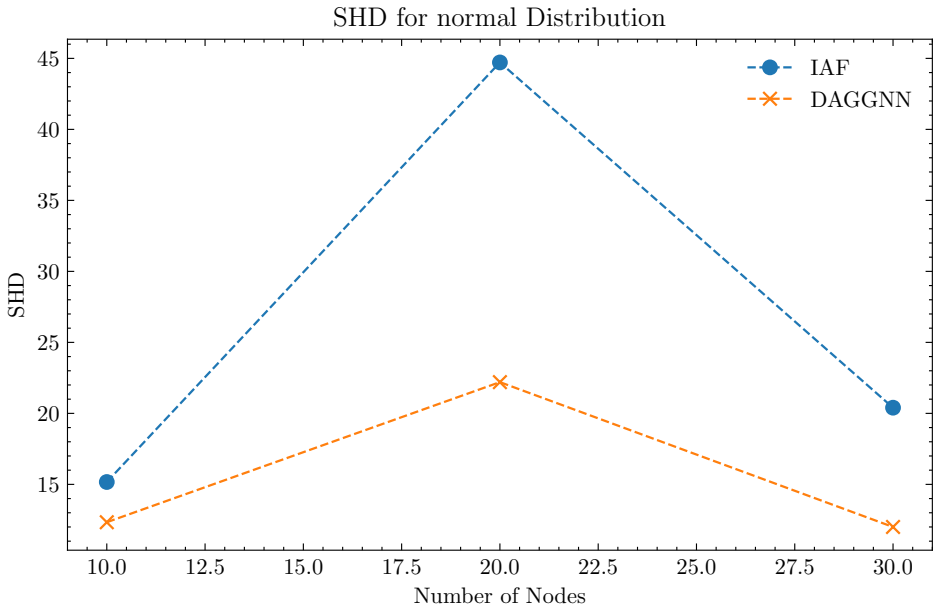

Figure: SHD with normal

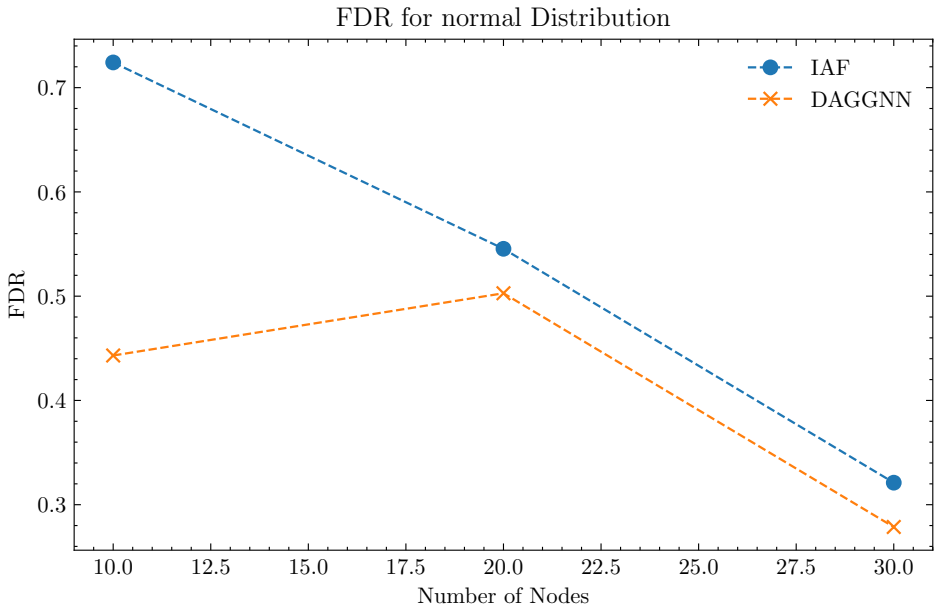

Figure: FDR with normal

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

Independent Noise (cont'd)

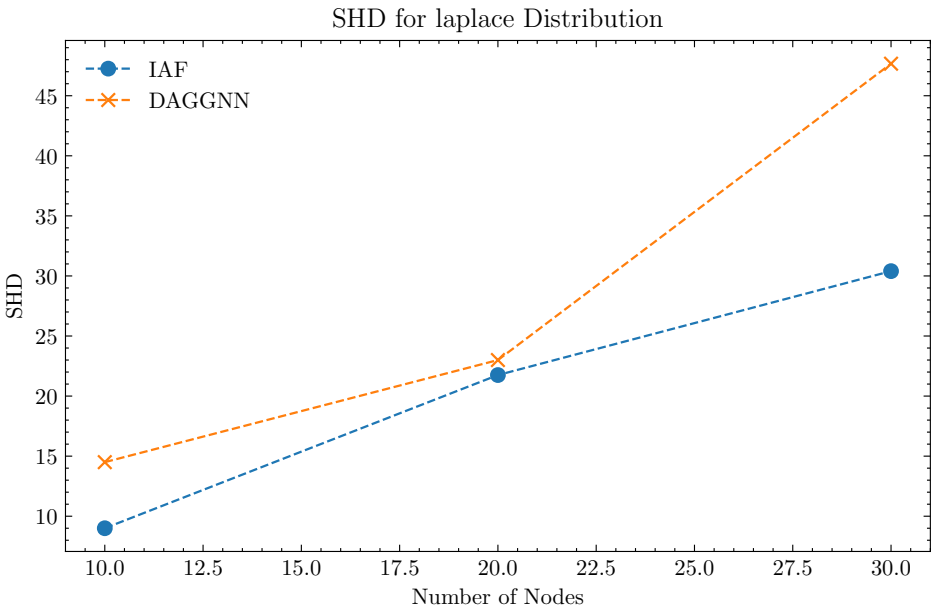

Figure: SHD with Laplace

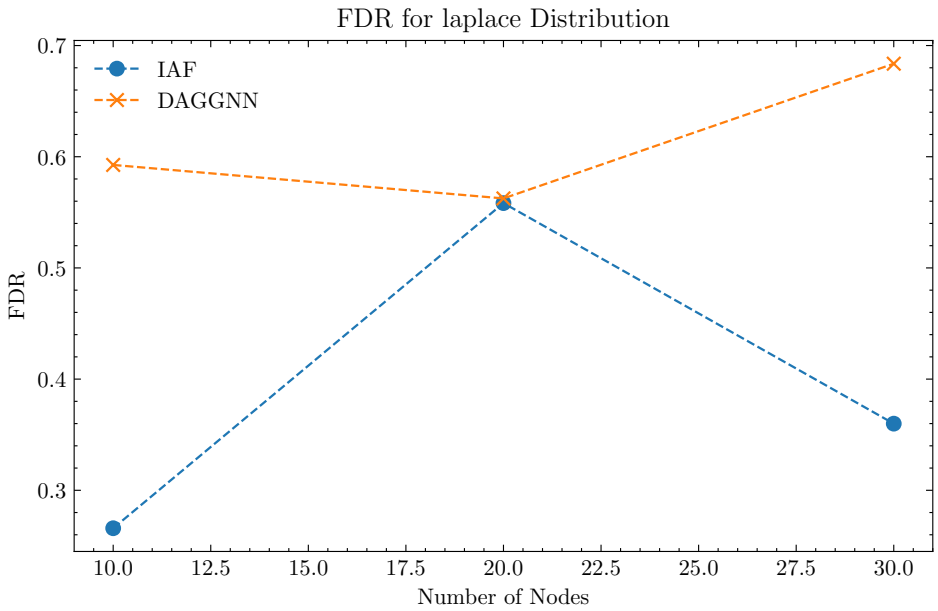

Figure: FDR with Laplace

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

Independent Noise (cont'd)

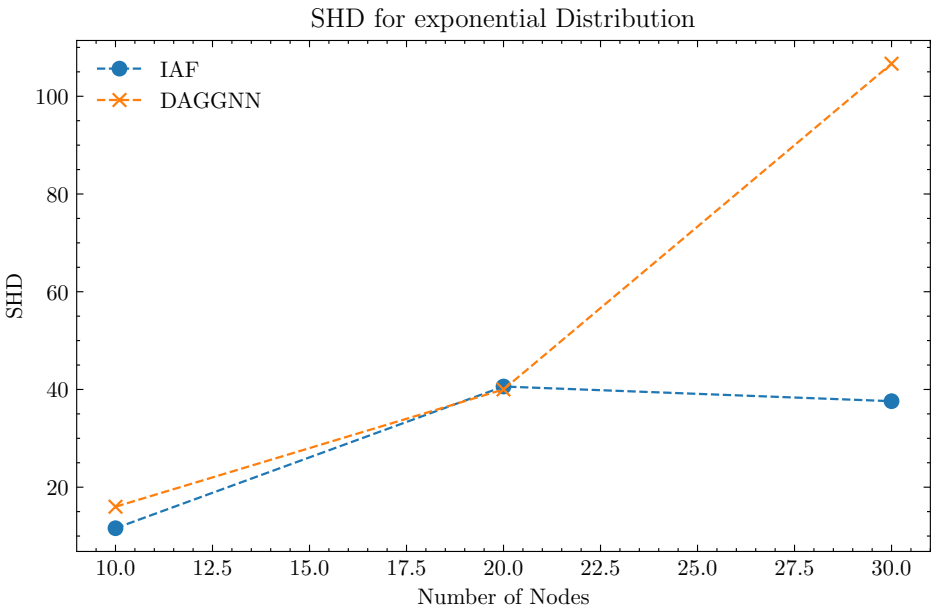

Figure: SHD with Exponential

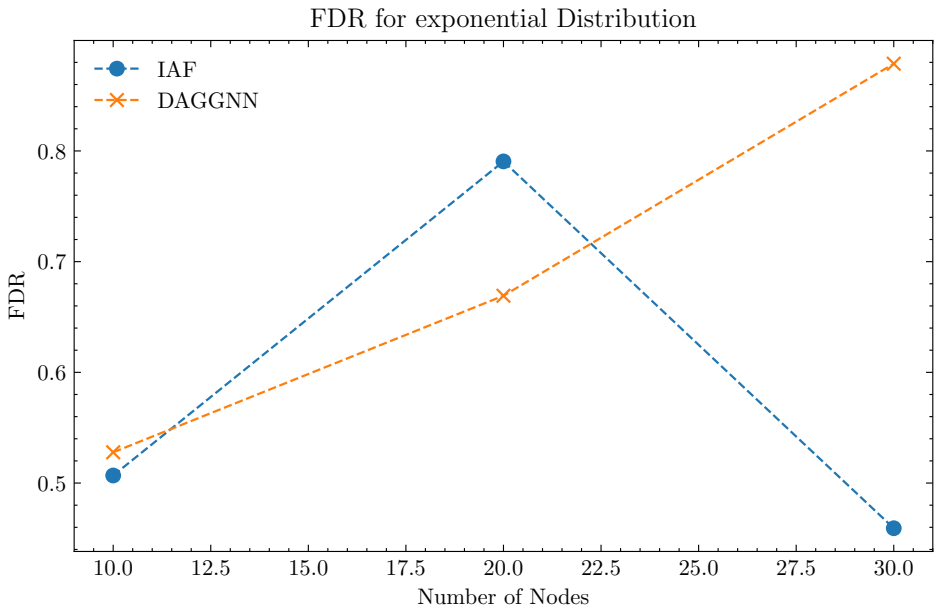

Figure: FDR with Exponential

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

Independent Noise (cont'd)

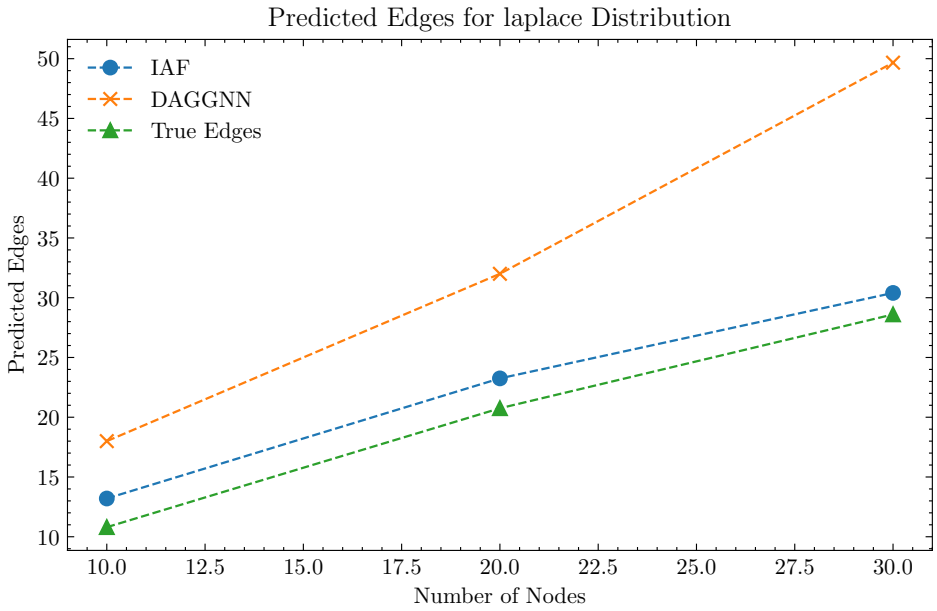

Figure: Number of predicted edges with Laplace

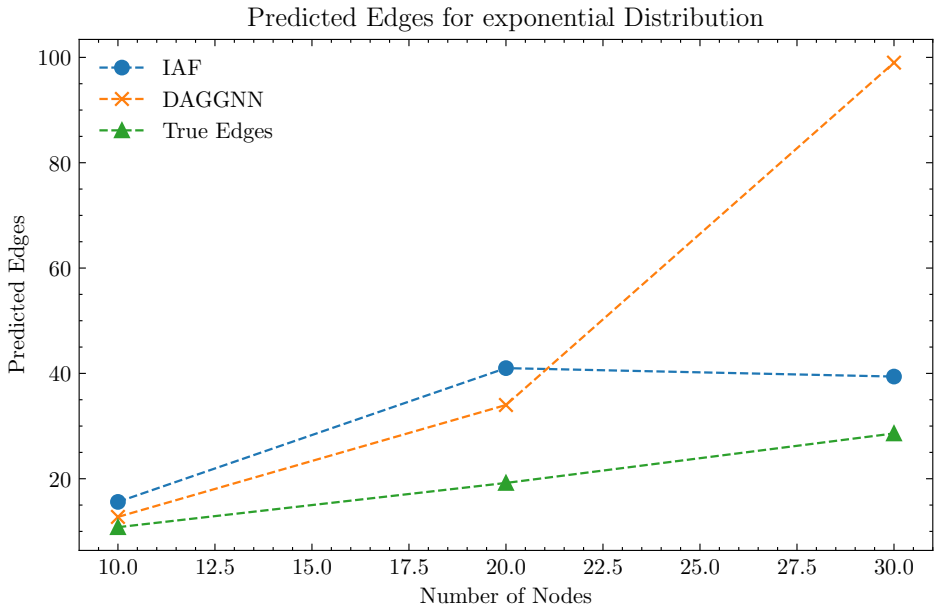

Figure: Number of predicted edges with Exponential

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

Independent Noise (cont'd)

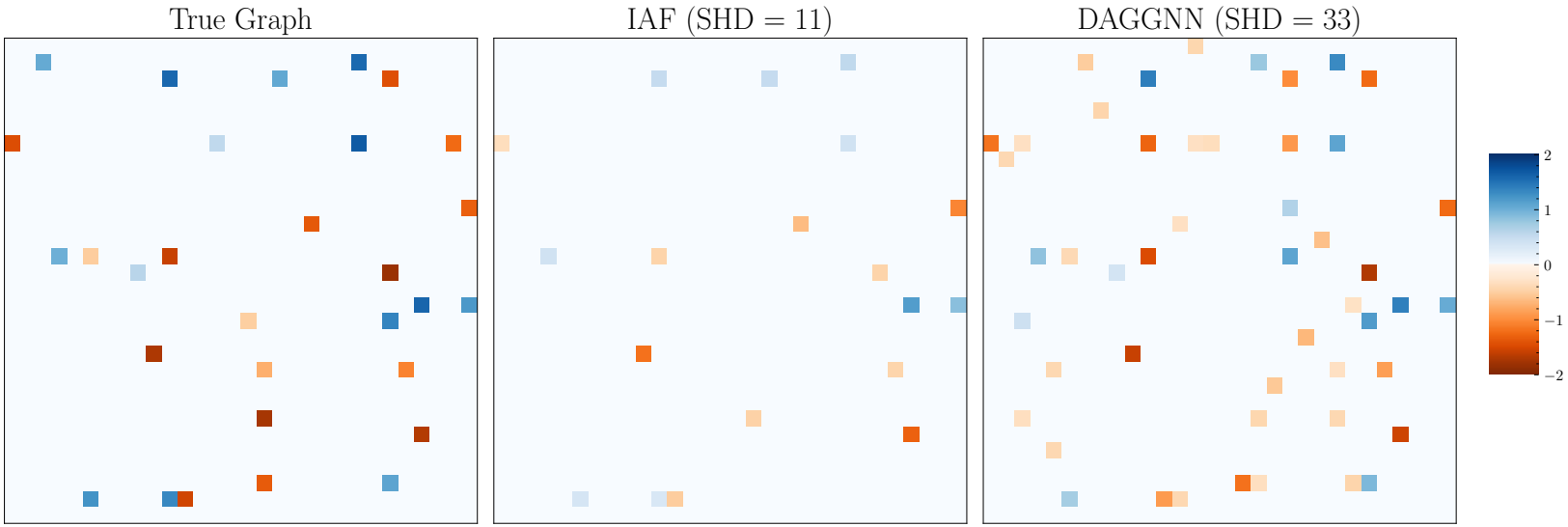

Figure: Comparison of estimated graphs with Laplace noise

Independent Noise (cont'd)

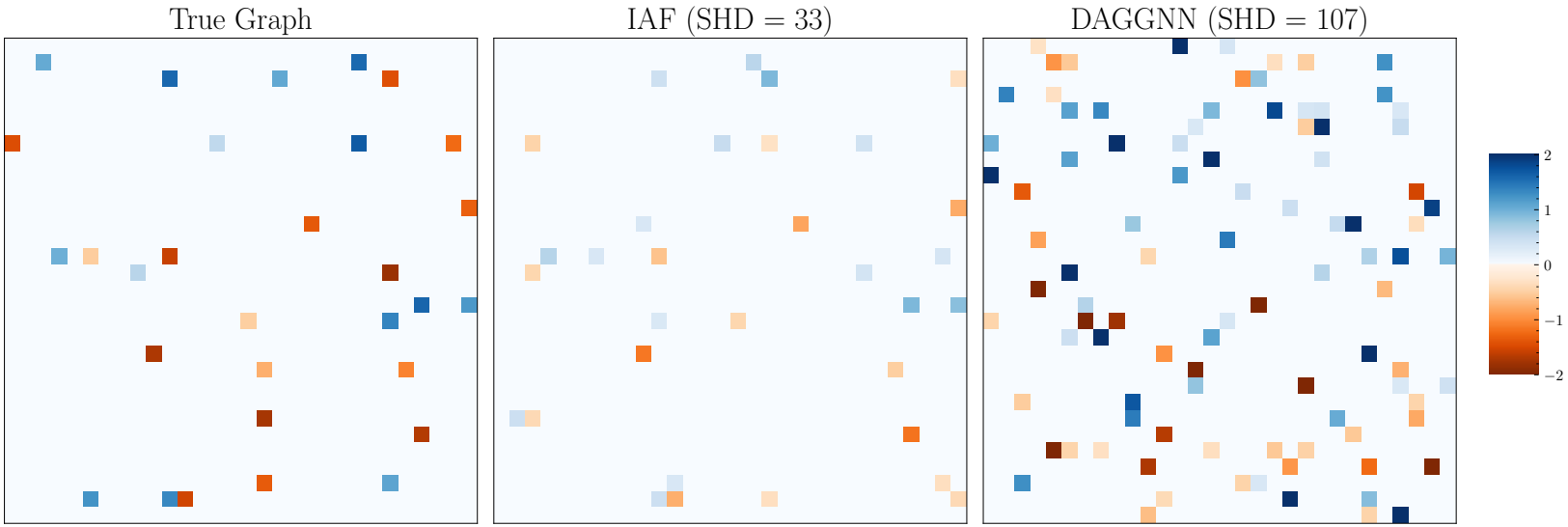

Figure: Comparison of estimated graphs with Exponential noise

Dependent Noise

Proportion of bidirectional edges fixed to 0.3.

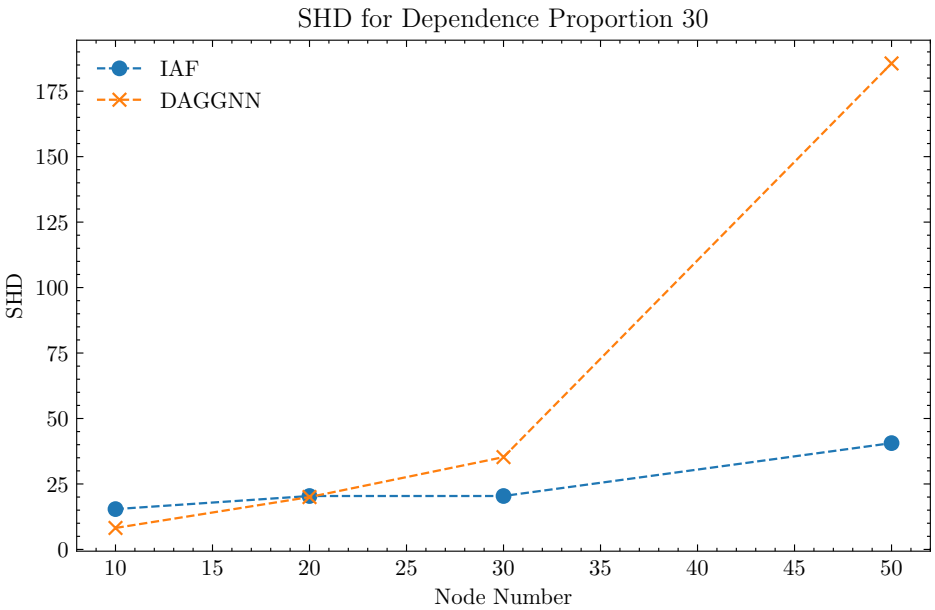

Figure: SHD with dependent Gaussian

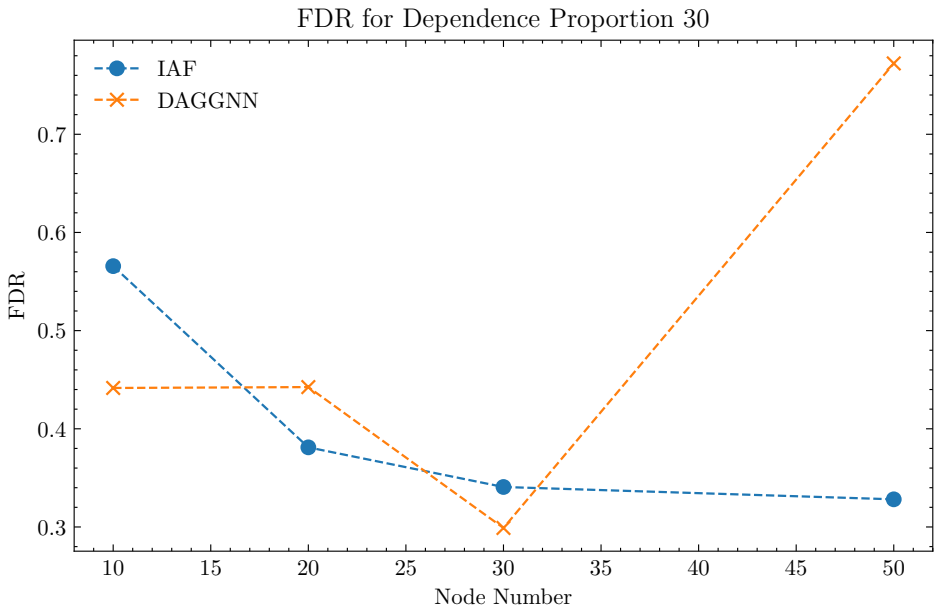

Figure: FDR with dependent Gaussian

Proportion of bidirectional edges fixed to 0.3.

Dependent Noise (cont'd)

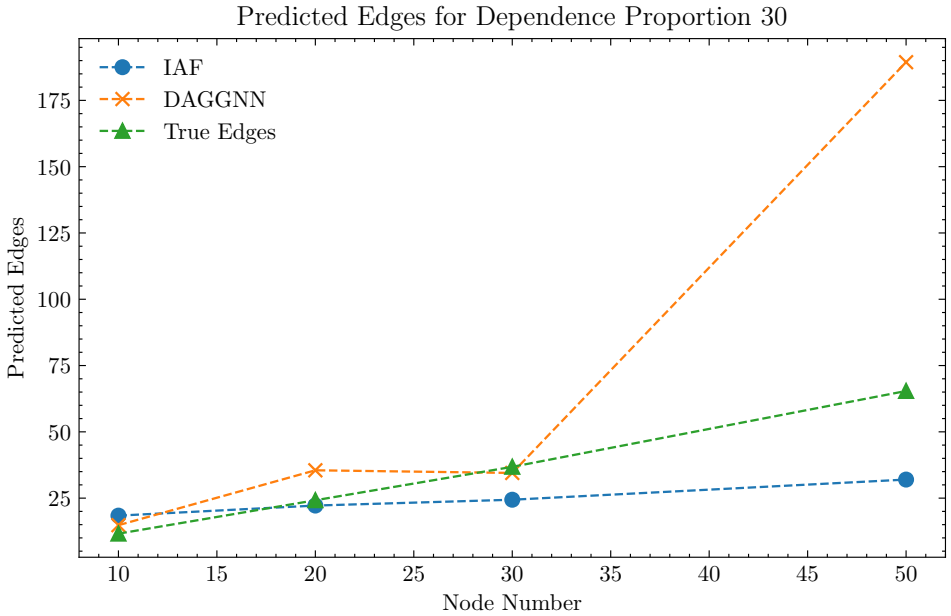

Figure: Number of predicted edges with dependent Gaussian

- 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).

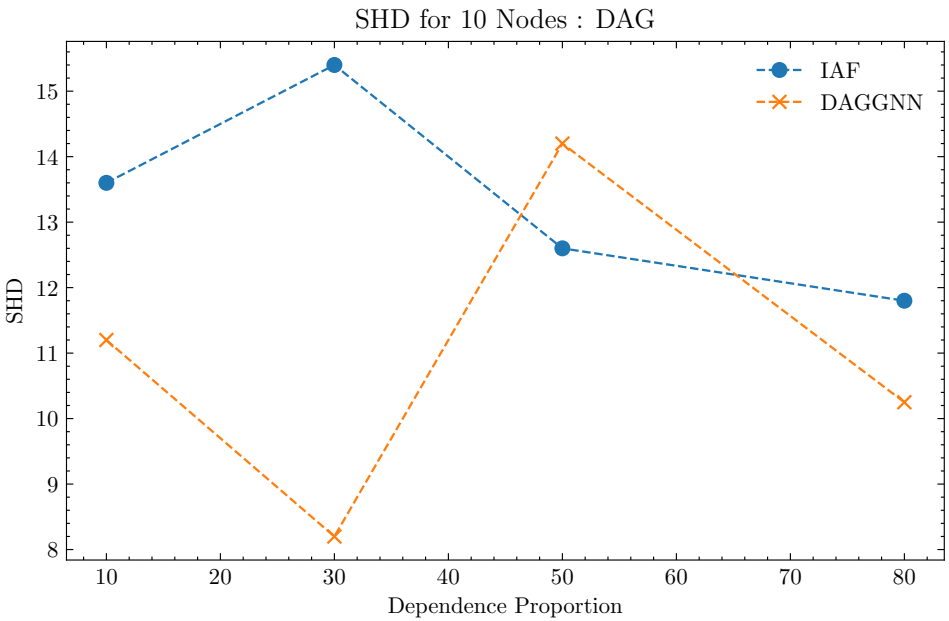

Figure: SHD with dependent Gaussian

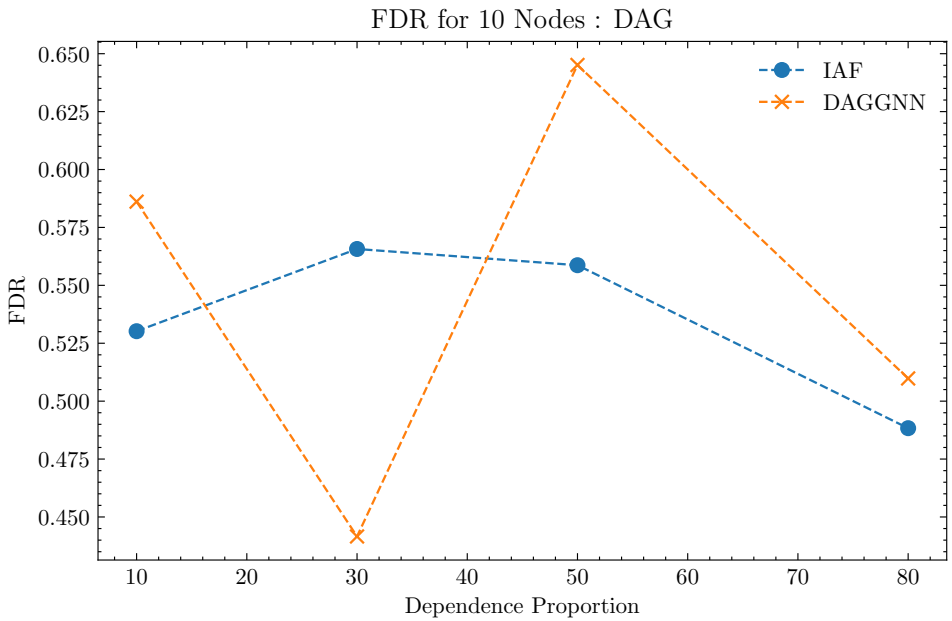

Figure: FDR with dependent Gaussian

Dependent Noise (cont'd)

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

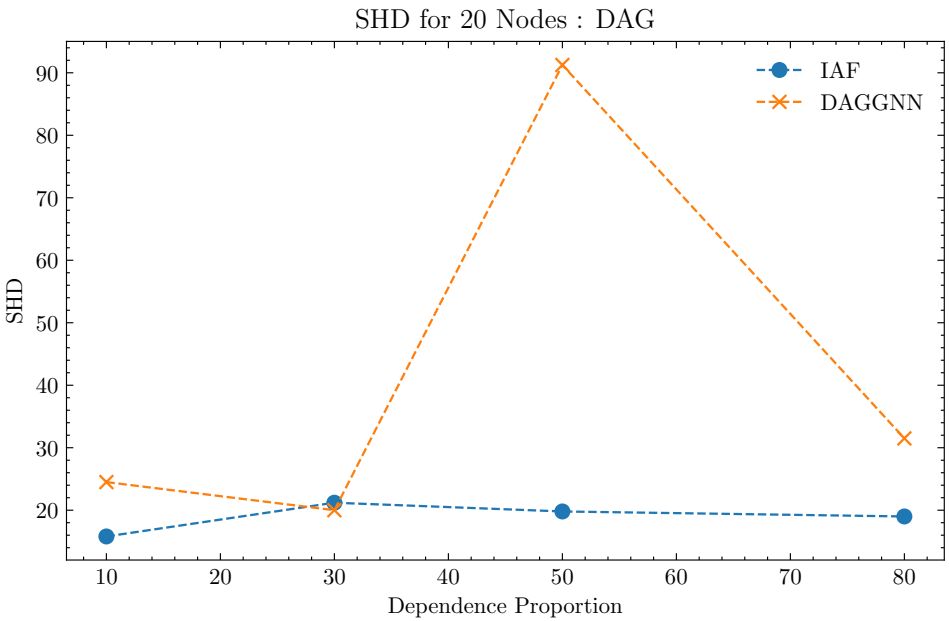

Figure: SHD with dependent Gaussian

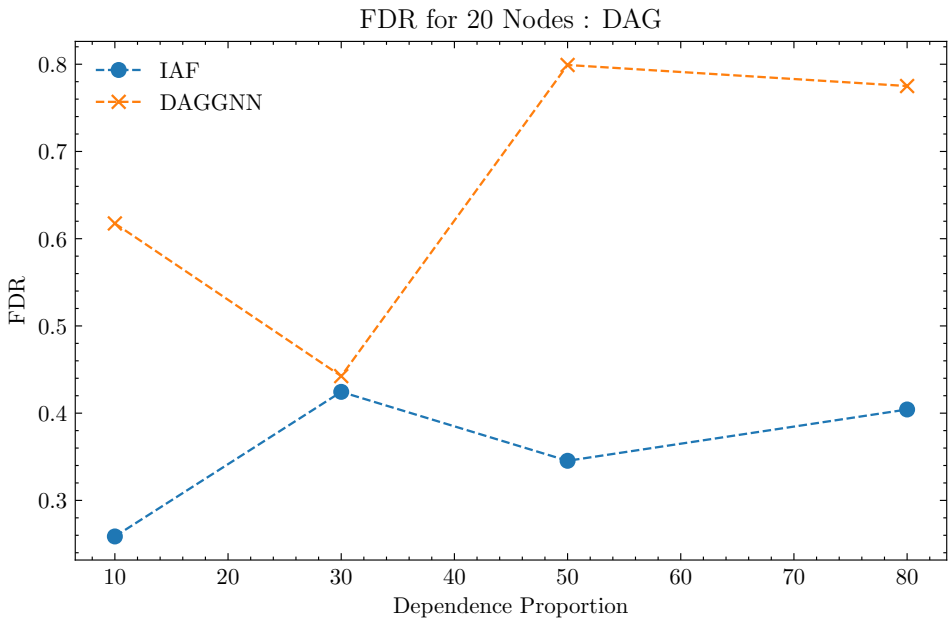

Figure: FDR with dependent Gaussian

Dependent Noise (cont'd)

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

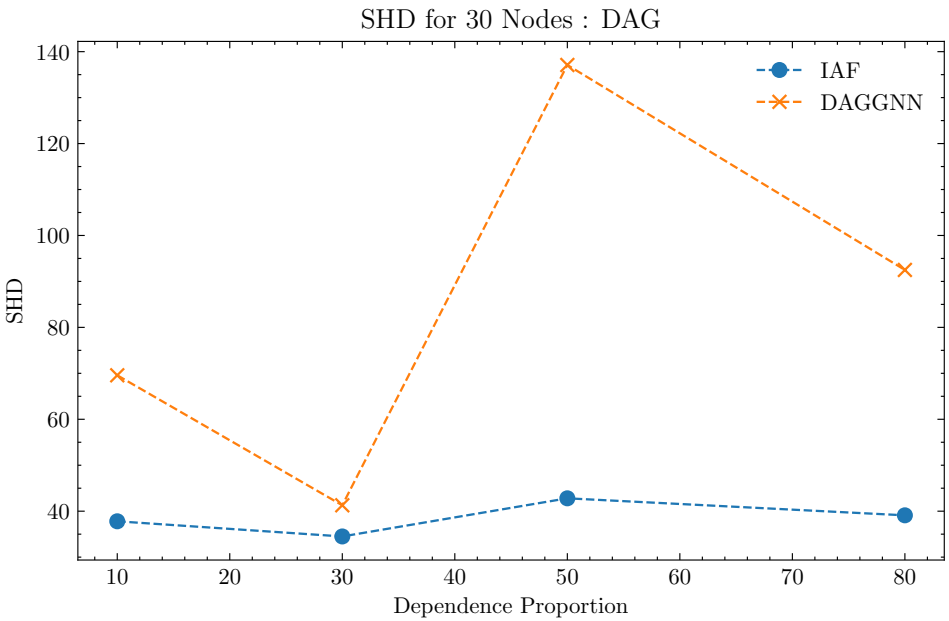

Figure: SHD with dependent Gaussian

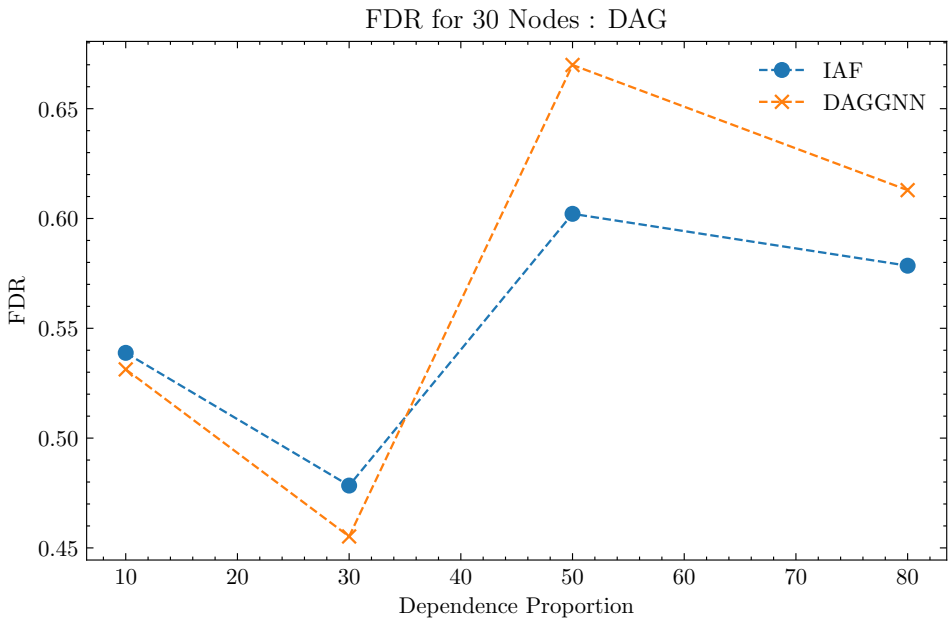

Figure: FDR with dependent Gaussian

Dependent Noise (cont'd)

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

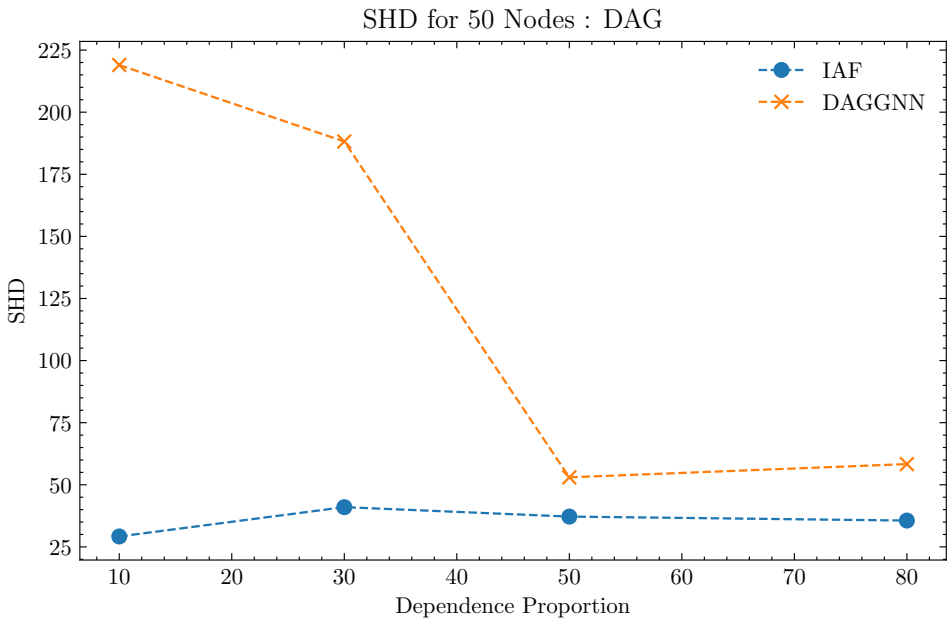

Figure: SHD with dependent Gaussian

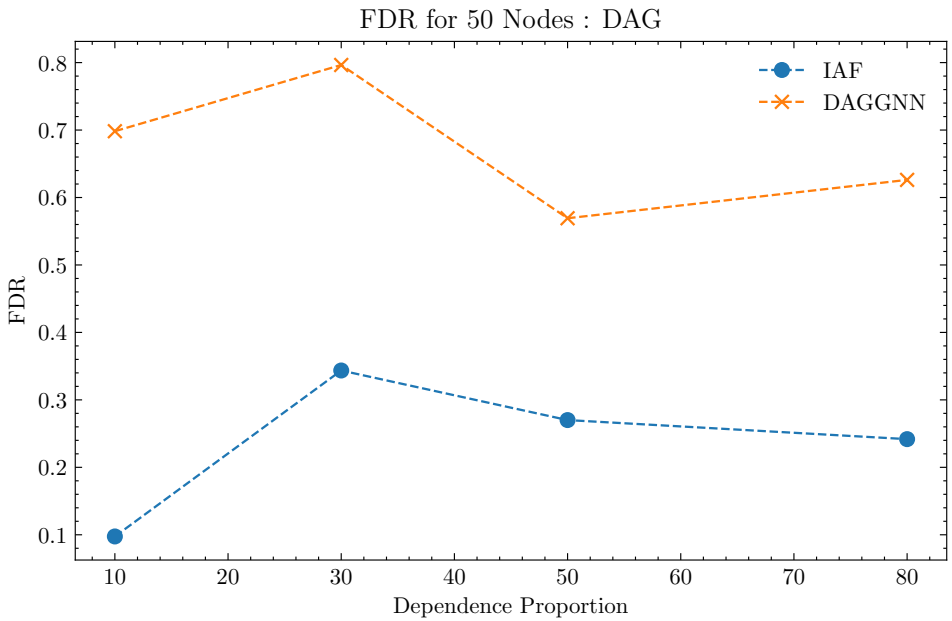

Figure: FDR with dependent Gaussian

Dependent Noise (cont'd)

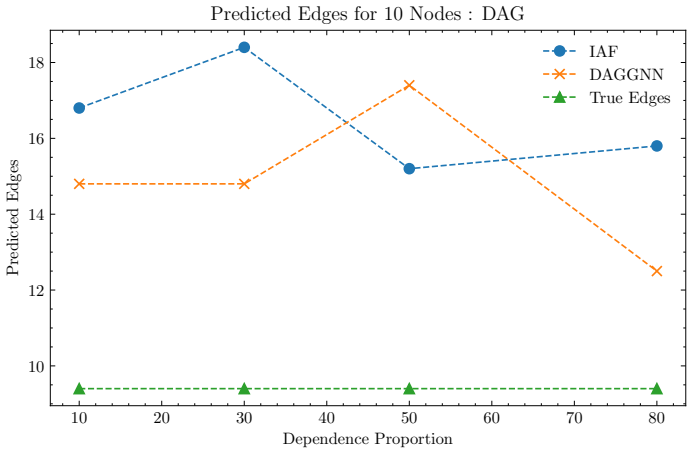

Figure: $m = 10$

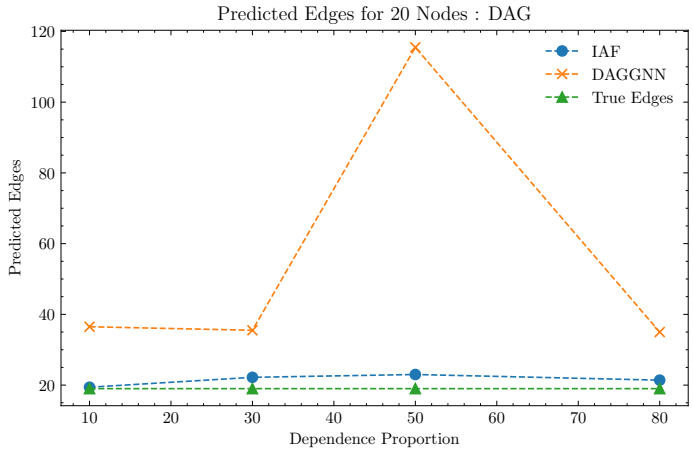

Figure: $m = 20$

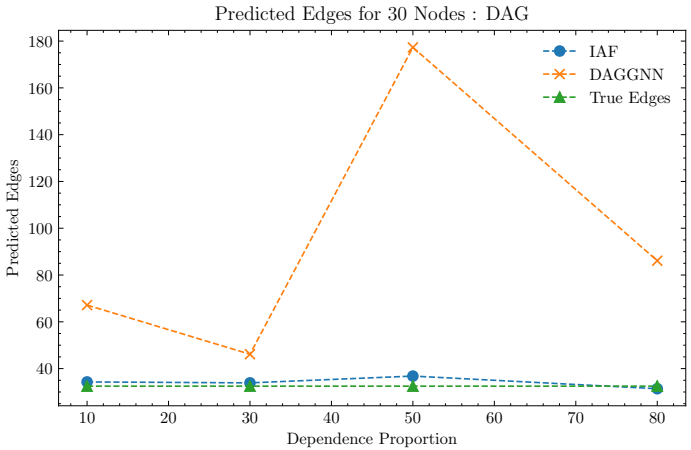

Figure: $m = 30$

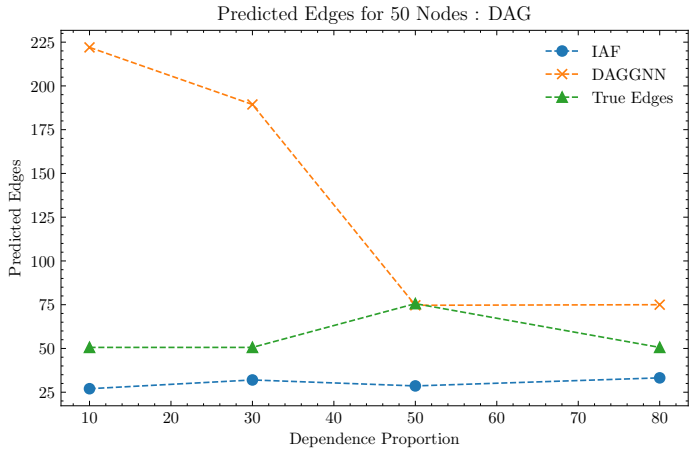

Figure: $m = 50$

Dependent Noise (cont'd)

- FPR : our method performs better than DAG-GNN.
- TPR : similar performance

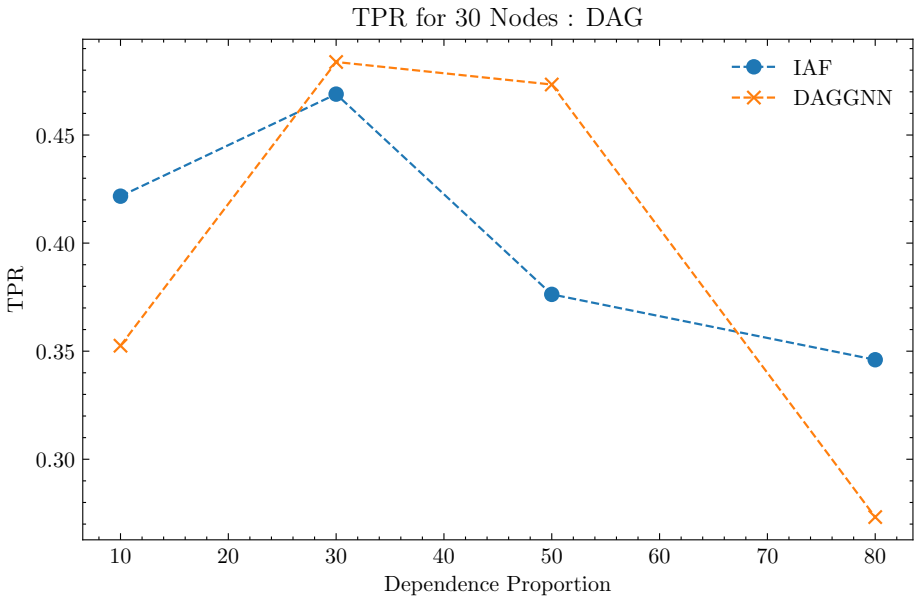

Figure: TPR at $m = 30$

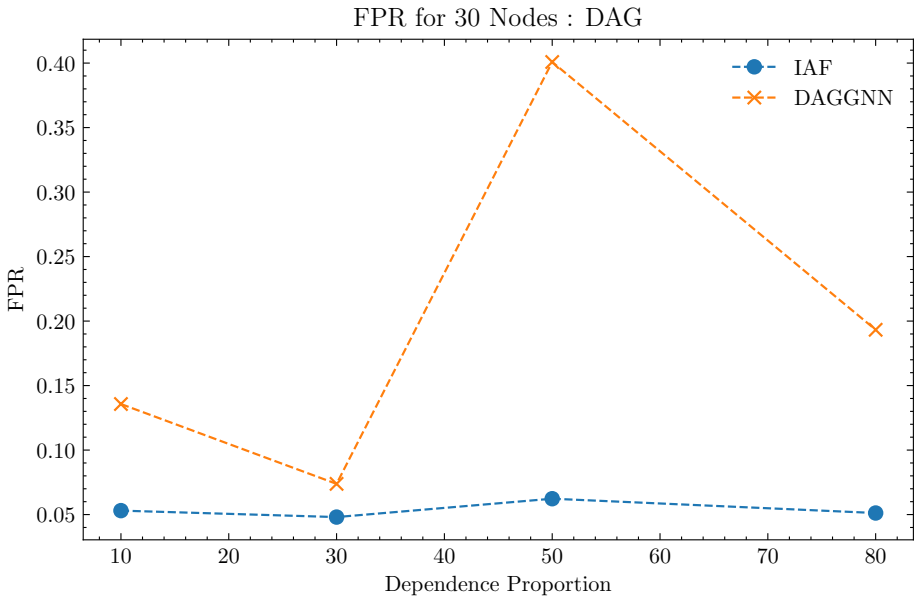

Figure: FPR at $m = 30$

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

- 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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