

# SUPPLEMENTARY MATERIALS FOR 'ALPHA-DAG: A REINFORCEMENT LEARNING BASED ALGORITHM TO LEARN DIRECTED ACYCLIC GRAPHS'

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## A PIPELINE OF ALPHA-DAG

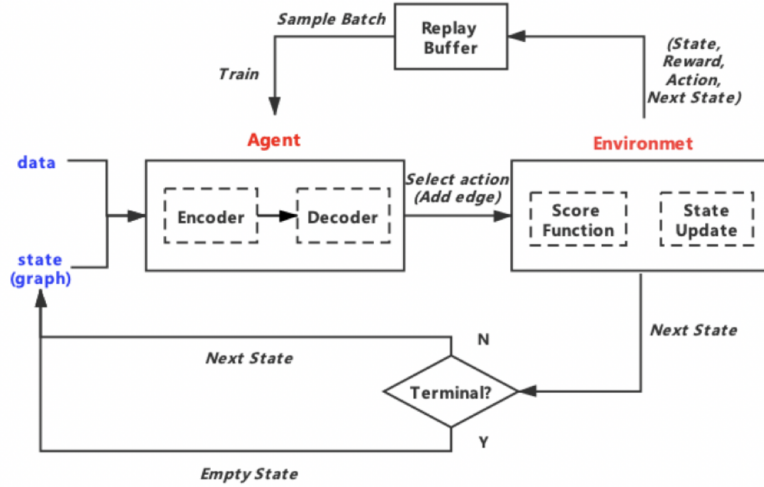


Figure 1: The main architecture of Alpha-DAG

## B MORE RESULTS FOR $d = 30$ LINEAR EXAMPLE

Figures 2 and 3 plot the change of FDR and TPR during the training process for AL1, AL2, RL1, RL2 from a randomly selected seed. Both AL1 and AL2 outperform RL1 and RL2 in the  $d = 30$  case. We can clearly see that the training curves of TPR and FDR by Alpha-DAG looks more reasonable than RL since RL fails to find a right direction to improve these two measurements.

## C LIENAR EXAMPLE WITH $p = 0.5$

In this section, we provide the additional numerical results for the linear model under dense graph case, with  $p = 0.5$ ,  $n = 256$  and  $d = 12$ .

Table 1: Empirical results on linear-Gaussian and linear-non-Gaussian data models with 12-node prob-0.5.

		AL1	AL2	RL1	RL2	CAM	DAG-GNN	GES	LINGAM	NOTEARS	PC
LiG	FDR	0.28±0.03	0.05±0.06	0.52±0.19	0.08±0.12	0.50±0.18	0.29±0.06	0.44±0.20	0.24±0.12	0.11±0.09	0.61±0.05
	TPR	0.73±0.15	1.00±0.00	0.34±0.13	0.99±0.02	0.46±0.25	0.75±0.05	0.45±0.21	0.67±0.10	0.80±0.09	0.12±0.03
	SHD	16.0±3.6	1.7±2.1	33.3±9.0	3.3±4.9	29.3±11.6	19.3±6.1	27.3±11.5	17.7±5.8	9.7±3.8	35.3±2.3
LiNG	FDR	0.28±0.09	0.04±0.06	0.54±0.21	0.08±0.09	0.56±0.10	0.30±0.08	0.50±0.08	0.20±0.09	0.15±0.08	0.54±0.12
	TPR	0.76±0.12	0.98±0.03	0.33±0.21	0.96±0.06	0.33±0.10	0.73±0.08	0.41±0.07	0.70±0.10	0.76±0.10	0.15±0.07
	SHD	15.3±6.3	2.2±3.1	31.2±8.5	4.0±4.8	34.2±5.1	20.8±6.6	30.7±3.8	14.7±6.1	11.3±4.4	32.8±2.2

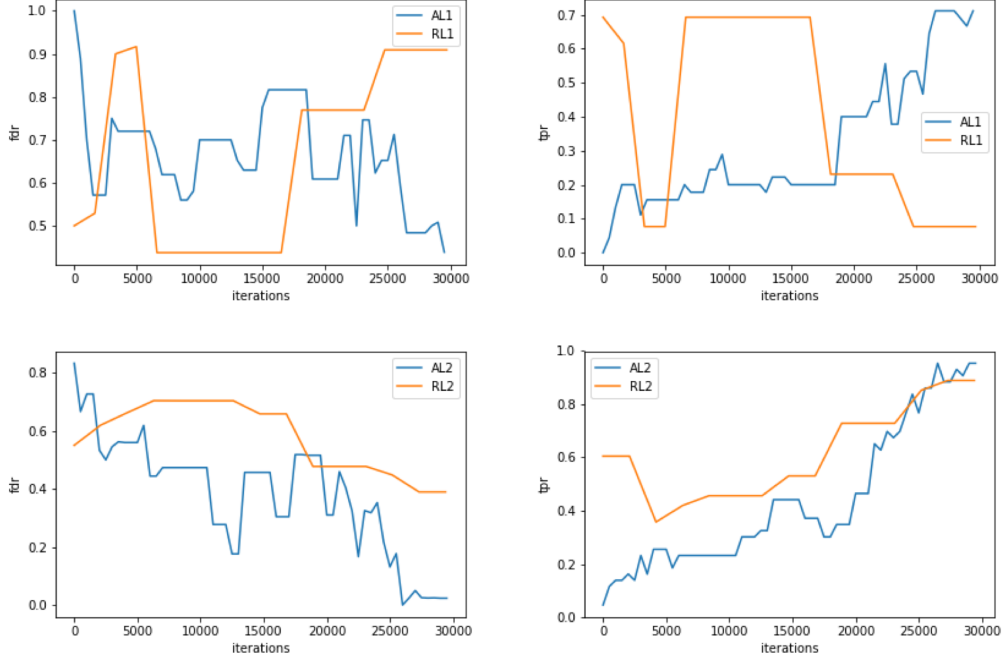


Figure 2: The change of FDR and TPR during the training process for AL1, AL2, RL1, RL2 in linear Gaussian case

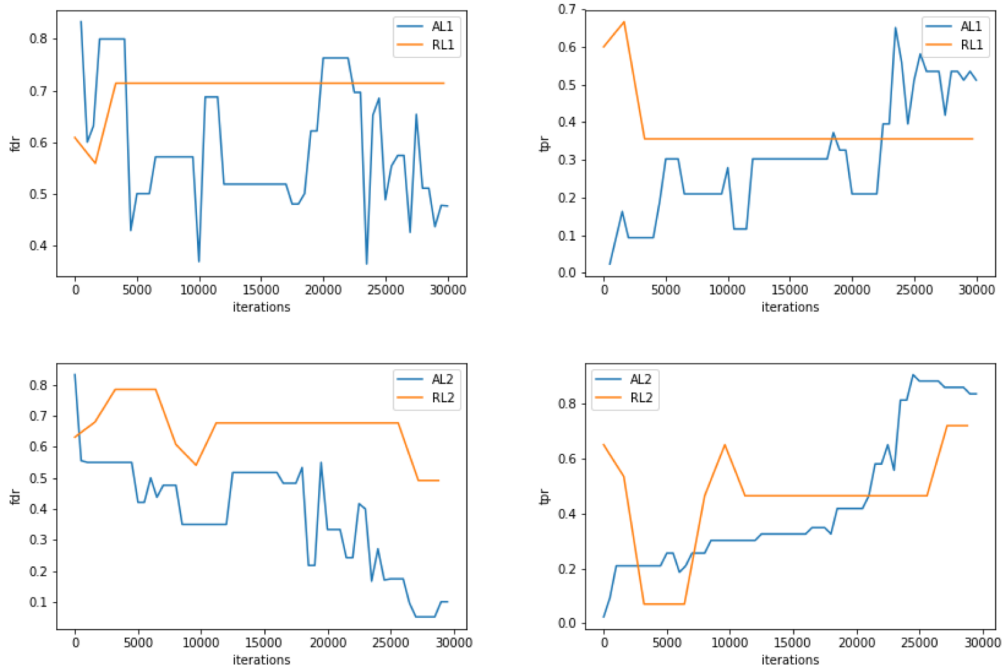


Figure 3: The change of FDR and TPR during the training process for AL1, AL2, RL1, RL2 in linear non-Gaussian case

## D IMPLEMENTATION DETAILS OF COMPETITORS

The implementation details of the other competitors are listed below:

1. LiNGAM (Shimizu et al., 2006). The method assumes linear non-Gaussian additive model and applies Independent Component Analysis (ICA) and thresholds on the weights to recover the weighted adjacency matrix. We use R package repository at <https://github.com/christinaheinze/CompareCausalNetworks>. We use `getParents` function to get the result graphs.
2. GES (Ramsey et al., 2017). The GES methods finds the result adjacency matrix by a two-phase greedy research. The method is available at <https://github.com/christinaheinze/CompareCausalNetworks>. We use `getParents` function to get the result graphs.
3. PC algorithm (Spirtes et al., 2000). The method is available at <https://github.com/christinaheinze/CompareCausalNetworks>. We use `getParents` function to get the result graphs.
4. CAM (Peters et al., 2014). The method decouples the causal order search among the variables from feature or edge selection in a DAG. Codes are available through <https://github.com/christinaheinze/CompareCausalNetworks>. We use `getParents` function to get the result graphs.
5. NOTEARS (Zheng et al., 2018). The methods recovers the causal graph by estimating the weighted adjacency matrix with the least squares loss and the smooth characterization for acyclicity constraint and thresholds on the weights. Codes are available at <https://github.com/xunzheng/notears>.
6. DAG-GNN (Yu et al., 2019). The methods formulates causal discovery in the framework of variational autoencoder, where the encoder and decoder are two shallow graph NNs. With a modified smooth characterization on acyclicity, DAG-GNN optimizes a weighted adjacency matrix with the evidence lower bound as loss function. Python codes are available at repository <https://github.com/fishmoon1234/DAG-GNN>.
7. RL (Zhu & Chen, 2019). This algorithms is a encoder-decoder model to search for the DAG with the best scoring based on reinforce learning framework. The implementation is available at [https://github.com/huawei-noah/trustworthyAI/tree/master/Causal\\_Structure\\_Learning/Causal\\_Discovery\\_RL](https://github.com/huawei-noah/trustworthyAI/tree/master/Causal_Structure_Learning/Causal_Discovery_RL).

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