Redefining the Shortest Path Problem Formulation of the Linear Non-Gaussian Acyclic Model: Pairwise Likelihood Ratios, Prior Knowledge, and Path Enumeration

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Outline

1. Towards LiNGAM as a Shortest Path Problem (LiNGAM-SPP)
   - Graphical Causality
   - Linear Non-Gaussian Acyclic Models (LiNGAM)
   - LiNGAM-SPP
2. **Improving LiNGAM-SPP** using Pairwise Likelihood Ratios
   - Tests on Simulated Data
   - Tests on Real-world Datasets
3. **Extension 1: Incorporating Known Relative Ordering** via a node-skipping strategy
4. **Extension 2: Predicting Causal Graph Properties**
   - Utilizing the Path Distribution of all Causal Orderings
   - Predicting Confounder Presence
   - Predicting Causal Graph Sparseness
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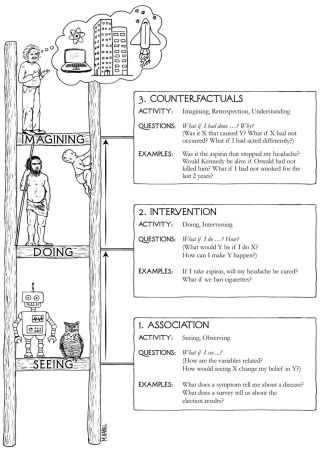
Graphical Causality



Pearl & Mackenzie (2018)

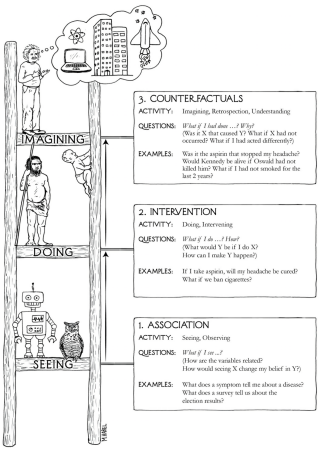
- Level 1: Association
- Level 2: Interventions
  - Do-calculus, e.g. $P(Y|do(X = x))$
  - Given some causal graph $\mathcal{G}$:

$$P(X_1, \ldots, X_n) = \prod_{i=1}^{n} P(X_i|\mathrm{PA}_i^{\mathcal{G}})$$

  - e.g. Average Treatment Effects
- Level 3: Counterfactuals
  - e.g. $PNS = P(Y_{X=0} = 0, Y_{X=1} = 1)$
  - Uses Structural Causal Models (SCMs). For some causal graph $\mathcal{G}$

$$X_i := f_i(\mathrm{PA}_i^{\mathcal{G}}, U_i).$$

Graphical Causality



Pearl & Mackenzie (2018)

- Causal Inference
  - Given a *causal graph* and data, estimate causal quantities.
- **Causal Discovery**
  - Given data (observational or interventional), learn the underlying *causal graph*.
  - relies of assumptions about the data generating process
  - e.g. causal faithfulness, structural form like Additive Noise Models and **LiNGAM**

Linear Non-Gaussian Acyclic Models (LiNGAM)

- SCM restricted to linear models and non-Gaussian noise:

$$\mathbf{x} = \mathbf{B}\mathbf{x} + \mathbf{e}$$

- Algorithms/ Methods:
  - ICA-LiNGAM (Shimizu et al. (2006))
  - **DirectLiNGAM** (Shimizu et al. (2011))

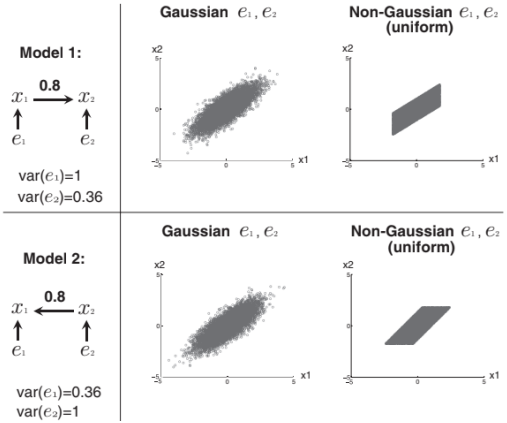


Figure from Shimizu (2014).

Linear Non-Gaussian Acyclic Models (LiNGAM)

- DirectLiNGAM steps:
  1. Get the **causal order**.
  2. Remove edges with adaptive lasso.
- e.g. The the causal ordering of $\{X, Y, Z\}$, we get a fully connected DAG

$$\begin{cases} X := \epsilon_1 \\ Y := aX + \epsilon_2 \\ Z := bX + cY + \epsilon_3 \end{cases}$$

- We can think of DirectLiNGAM as a *greedy algorithm* that determines the causal order in a fixed number of steps.

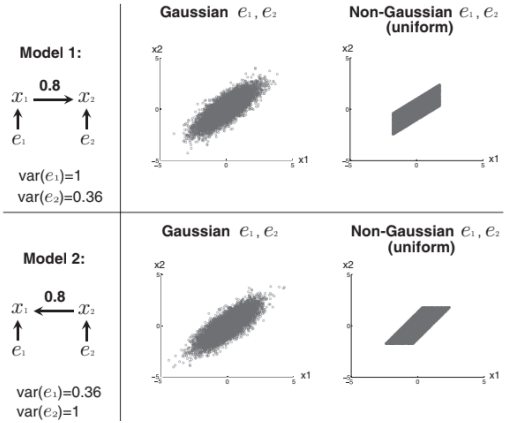


Figure from Shimizu (2014).

Linear Non-Gaussian Acyclic Models (LiNGAM)

DirectLiNGAM

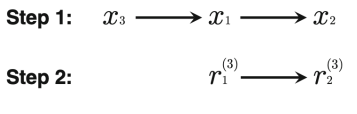


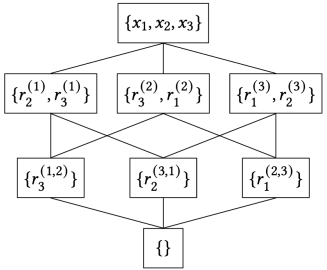
Figure 7: An illustration of DirectLiNGAM: $r_2^{(3,1)}$ denotes the residual when $r_2^{(3)}$ is regressed on $r_1^{(3)}$.

Figure from Shimizu (2014)

$$r_i^{(j)} = x_i - \frac{cov(x_i, x_j)}{var(x_j)} x_j$$

$$\begin{cases} x_3 := \epsilon_3 \\ x_1 := \alpha x_3 + \epsilon_1 \implies r_1^{(3)} = x1 - \alpha x_3 \\ x_2 := \beta x_1 + \gamma x_3 + \epsilon_2 \implies r_2^{(3)} = x_2 - \gamma x_3 \end{cases}$$

LiNGAM as a Shortest Path Problem (LiNGAM-SPP)



Adapted from Suzuki & Yang (2022).

- Each of the $n!$ paths corresponds to a causal ordering
- This takes advantage of the property:

$$I(X, Y, Z) = I(\{X, Y\}, Z) + I(X, Y)$$

- The path $\{x_1, x_2, x_3\} \rightarrow \{r_2^{(1)}, r_3^{(1)}\} \rightarrow \{r_3^{(1,2)}\} \rightarrow \{\}$ corresponds to the causal ordering $\{X_1, X_2, X_3\}$ and is computed by adding the edges

$$I(\epsilon_1, \epsilon_2, \epsilon_3) = I(x_1, \{r_2^{(1)}, r_3^{(1)}\}) + I(r_2^{(1)}, r_3^{(1,2)}) + 0$$

- Dijkstra's algorithm with lazy evaluation was used.

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Improving LiNGAM-SPP

- The initial LiNGAM-SPP paper used a kNN-based mutual information estimator. (Suzuki & Yang (2022))
- A subsequent study used Copula Entropy. (Suzuki & Yang (2024))
- Both methods relied on tuning the k parameter.
- We propose using **Pairwise Likelihood Ratios (PLR)** instead. (Hyvärinen & Smith (2013)). PLR doesn't require parameter tuning.
- We adapted the PLR implementation from the `lingam` package. (Ikeuchi et al. (2023))

Tests on Simulated Data

We compare the following methods:

- PLR LiNGAM-SPP (our method)
- PLR DirectLiNGAM (default implementation in `lingam` package)
- Copent LiNGAM-SPP* (from Suzuki & Yang (2024))
- kNN LiNGAM-SPP* (from Suzuki & Yang (2022))

Using the ordering error as the metric:

$$E_o = \frac{2r}{p(p-1)},$$

where p represents the number of features and r is the count of pairs in the wrong order.

*for the sake of comparison, we take the best performing k among $0.05N$, $0.1N$, and $\sqrt{N}$ where N is the sample size of the simulation.

Steps to Generate Simulations

This was patterned after Shimizu et al. (2011), modified to include confounders.

1. We initialized the matrix $\mathbf{B}$ by creating a $p \times p$ lower triangular matrix with elements randomly drawn from a uniform distribution in the interval $[-1.5, -0.5] \cup [0.5, 1.5]$, following Silva et al. (2006).
2. To introduce sparsity into the graph, we applied an element-wise product with a Bernoulli distribution matrix, following the approach of Kalisch & Bühlmann (2007). The success probability parameter of this Bernoulli distribution determines the sparseness of the graph.
3. For modeling non-Gaussian noise and confounders, we used the set of 18 non-Gaussian distributions used in Bach & Jordan (2003). Each noise term and confounder were randomly sampled from this set. Moreover, we scaled these distributions to ensure their variances fell within the interval $[1, 3]$, as in Silva et al. (2006).
4. Construct $\mathbf{\Lambda}$ sequentially. Me make sure that each confounder must confound at least 2 variables and that no 2 confounders can confound the same set of variables.

Simulation Results: Average Ordering Error

		Without Confounders				With Confounders			
	Sample Size (N)	100	250	500	1000	100	250	500	1000
p	Method								
5	PLR LiNGAM-SPP	0.29	0.28	0.23	0.21	0.46	0.45	0.42	0.39
	PLR DirectLiNGAM	0.29	0.28	0.23	0.22	0.46	0.45	0.42	0.40
	Copent LiNGAM-SPP	0.40	0.41	0.38	0.39	0.43	0.40	0.43	0.42
	*k*NN LiNGAM-SPP	**0.29**	**0.23**	**0.22**	**0.18**	**0.40**	**0.37**	**0.35**	**0.33**
10	PLR LiNGAM-SPP	0.33	**0.24**	**0.21**	**0.18**	0.44	**0.40**	**0.37**	**0.34**
	PLR DirectLiNGAM	**0.32**	0.25	0.22	0.19	**0.44**	0.41	0.37	0.36
	Copent LiNGAM-SPP	0.49	0.48	0.50	0.49	0.46	0.46	0.45	0.46
	*k*NN LiNGAM-SPP	0.48	0.40	0.35	0.30	0.49	0.43	0.39	0.35
15	PLR LiNGAM-SPP	0.33	**0.24**	**0.19**	**0.16**	**0.41**	**0.36**	0.35	**0.29**
	PLR DirectLiNGAM	**0.32**	0.25	0.21	0.18	0.42	0.37	**0.33**	0.32
	Copent LiNGAM-SPP	0.51	0.50	0.51	0.52	0.48	0.48	0.49	0.49
	*k*NN LiNGAM-SPP	0.56	0.51	0.45	0.38	0.54	0.49	0.46	0.40

Simulation Results: Average Runtime

		Without Confounders				With Confounders			
	Sample Size (N)	100	250	500	1000	100	250	500	1000
p	Method								
5	PLR LiNGAM-SPP	0.44s	0.44s	0.45s	0.46s	0.43s	0.45s	0.44s	0.46s
	PLR DirectLiNGAM	0.04s	0.04s	0.04s	0.05s	0.04s	0.04s	0.04s	0.05s
	Copent LiNGAM-SPP	0.06s	0.11s	0.3s	1.1s	0.07s	0.13s	0.35s	1.3s
	kNN LiNGAM-SPP	0.27s	0.39s	0.72s	1.8s	0.26s	0.37s	0.65s	1.7s
10	PLR LiNGAM-SPP	6.8s	6.9s	6.9s	6.1s	6.4s	7.2s	7s	7.6s
	PLR DirectLiNGAM	0.26s	0.27s	0.3s	0.36s	0.26s	0.27s	0.31s	0.36s
	Copent LiNGAM-SPP	0.4s	0.6s	1.3s	4.6s	0.48s	0.7s	1.6s	5.5s
	kNN LiNGAM-SPP	32s	45s	1.4m	3.5m	32s	44s	1.3m	3.4m
15	PLR LiNGAM-SPP	2.2m	1.6m	1.2m	1.5m	1.4m	3.6m	2.8m	3.2m
	PLR DirectLiNGAM	0.83s	0.9s	0.98s	1.2s	0.84s	0.92s	1s	1.2s
	Copent LiNGAM-SPP	1.3s	1.8s	3.4s	11s	1.6s	2.1s	4.3s	14s
	kNN LiNGAM-SPP	37m	48m	84m	206m	36m	49m	85m	205m

Tests on Real-World Datasets

- We use the following datasets from the CMU CLeaR Group:
  - sachs (Sachs et al. (2005))
  - yacht-hydrodynamics (Gerritsma et al. (2013))
  - abalone (Nash et al. (1995))
  - airfoil-self-noise (Brooks et al. (2014))
  - wine-quality-red (Cortez et al. (2009))
  - wine-quality-white (Cortez et al. (2009))
- LiNGAM-SPP is only concerned with causal ordering, we used the same sparse regression technique as DirectLiNGAM for edge removal.
- Ground Truth contains information on required and forbidden edges.

Results on CMU-CleaR Data

		Known Edges		DirectLiNGAM		LiNGAM-SPP	
Dataset	p	Req.	Forb.	Req.	Forb.	Req.	Forb.
sachs	11	20	0	10	0	10	0
yacht-hydrodynamics	7	1	15	0	2	0	2
abalone	8	0	17	0	4	0	4
airfoil-self-noise	6	0	11	0	6	0	6
wine-quality-red	12	2	11	1	7	2	2
wine-quality-white	12	2	11	2	4	2	1

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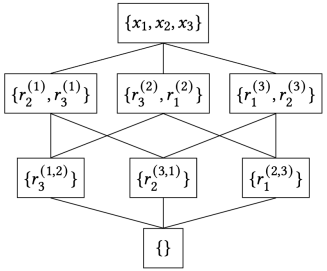
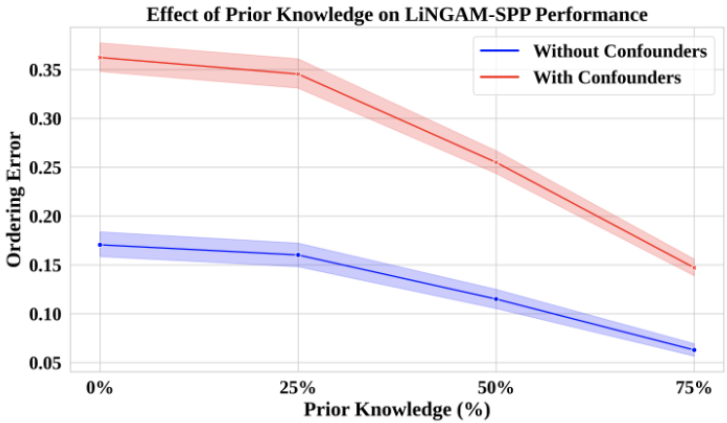
Incorporating Known Relative Ordering



Adapted from Suzuki & Yang (2022).

- In DirectLiNGAM, prior knowledge is given as an adjacency matrix where we specify edges as **required, forbidden, or unknown**.
- The path formulation allows for **relative ordering**, which is more flexible.
- Feature indices not in the subscripts are "earlier" in the ordering.
- e.g. if x_1 preceeds x_2, then the nodes with subscript 1 but not 2 ($\{r_3^{(2)}, r_1^{(2)}\}$ and $\{r_1^{(2,3)}\}$) should be skipped.

Results: Average Error vs Prior Knowledge

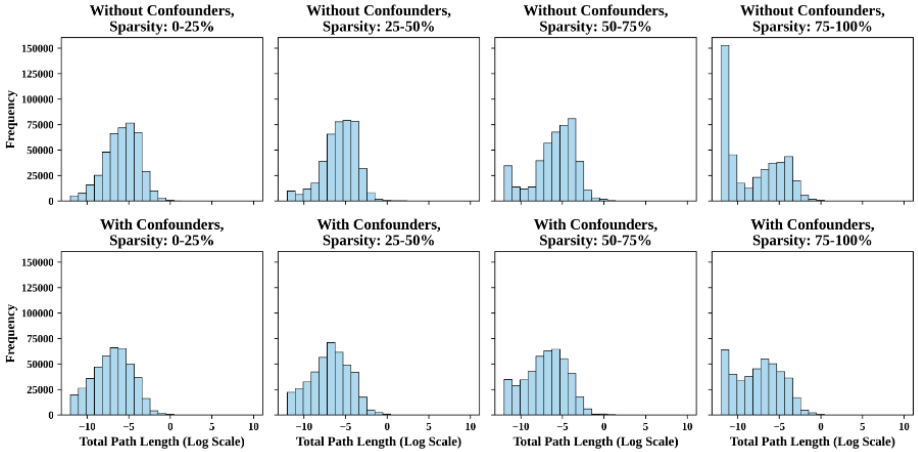


Combined results for $p = 4, 8, 12$.

Results: Computation Cost with Prior Knowledge

	Without Confounders				With Confounders			
Prior Knowledge p	0%	25%	50%	75%	0%	25%	50%	75%
4	9	9	8	6	9	9	8	6
8	35	34	27	18	39	40	37	22
12	107	99	81	42	184	198	174	74

Inspiration for Predicting Causal Graph Properties



Log-transformed Path Distributions for $p = 4, 5, 6$.

Predicting Using Path Distributions

- Use standardized moments to capture the shape of the distribution:

$$\tilde{\mu}_k = \frac{\mathrm{E}[(X-\mu)^k]}{(\mathrm{Var}[X-\mu])^{k/2}}.$$

- (Optional) Use ZDDs to enumerate path lengtths and compute moments. (see Lim et al. (Submitted))
- Use $p = 4, 5, 6$ for training and $p = 7$ to test.
- Create the following predictors:
  1. Confounder Detector - detect the presence of unmeasured confounders.
  2. Sparseness Estimator - estimate graph sparseness.
  3. Performance Predictors - predict the reliability of LiNGAM-SPP and DirectLiNGAM.

Predictor 1: Confounder Detector

Predict if unmeasured confounder is present.

Model	AUC	Precision	Recall	Accuracy	Optimal Threshold
*k*NN	0.6537	0.5918	0.7365	0.6142	0.4000
Random Forest	0.7608	0.6883	0.7465	0.7042	0.3300
XGBoost	0.7665	0.6955	0.7400	0.7080	0.3278
CatBoost	**0.7829**	**0.6957**	**0.7740**	**0.7178**	0.3271
AdaBoost	0.6997	0.6557	0.7540	0.6790	0.4972

Predictor 2: Sparseness Estimator

Predict if sparseness > 0.5.

Model	AUC	Precision	Recall	Accuracy	Optimal Threshold
*k*NN	0.6262	0.5949	0.6054	0.5905	0.4000
Random Forest	0.7286	0.7174	0.5640	0.6660	0.3400
XGBoost	0.7551	0.6773	**0.7443**	0.6902	0.2161
CatBoost	**0.7744**	0.7043	0.7217	**0.7050**	0.2647
AdaBoost	0.7579	**0.7285**	0.6438	0.6975	0.4958

Predictor 3: Performance Predictors

Predict if LiNGAM-SPP or DirectLiNGAM predicts the causal order correctly (i.e., $E_o = 0$).

	LiNGAM-SPP				DirectLiNGAM			
Model	AUC	Precision	Recall	Accuracy	AUC	Precision	Recall	Accuracy
*k*NN	0.641	0.155	0.613	0.617	0.638	0.147	0.594	0.615
Random Forest	0.822	0.272	0.752	0.768	**0.821**	0.239	**0.801**	0.725
XGBoost	0.799	0.237	**0.774**	0.721	0.800	**0.311**	0.648	**0.821**
CatBoost	**0.822**	**0.333**	0.698	**0.826**	**0.821**	0.306	0.711	0.809
AdaBoost	0.790	0.292	0.672	0.799	0.789	0.269	0.711	0.777

Conclusions

- Eliminated parameter tuning by replacing kNN-based estimators with PLR, improving performance and efficiency.
- PLR LiNGAM-SPP outperforms DirectLiNGAM in simulations and matches or exceeds its performance on real data.
- Incorporated prior knowledge with relative orderings, improving flexibility and performance.
- Developed confounder detector, sparsity estimator, and performance predictors using path distribution features, achieving high AUCs.

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