

CBMS Conference -- Foundations of Causal Graphical Models and Structure Discovery

Lecture 9

Causal Representation Learning: Recovery of the Hidden World

Instructor: Kun Zhang

Carnegie Mellon University



Outline

- Why causal/disentangled representations ?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Uncover Causality from Observational Data?



• Causal system has "irrelevant" modules (Pearl, 2000; Spirtes et al., 1993)



- conditional independence among variables;
- independent noise condition;
- minimal (and independent) changes...

Footprint of causality in data

- Causal discovery (Spirtes et al., 1993)/ causal representation learning (Schölkopf et al., 2021): find such representations with identifiability guarantees
- Three dimensions of the problem:

i.i.d. data?	Parametric constraints?	Latent confounders?					
Yes	No	No					
No	Yes	Yes					

Causal Representation Learning: A Summary

i.i.d. data?	Parametric constraints?	Latent confounders?	What can we get?						
	NLa	No	(Different types of)						
Vee	INO	Yes	equivalence class						
res	Vee	No	Unique identifiability						
	res	Yes	conditions)						
		No	(Extended) regression						
Non-I, but I.D.	NO/Yes	Yes	Latent temporal causal processes identifiable!						
	No	No	More informative than MEC (CD-NOD)						
	Yes	INO	May have unique identifiability						
I., DUL HOH-I.D.	No	Vee	Changing subspace identifiable						
	Yes	Tes	Variables in changing relations identifiable						

A Problem in Psychology: Finding Underlying Mental Conditions?

• 50 questions for big 5 personality test

race	age	engnat	gender	hand	source	country	E1	E2	E3	E4	E 5	E 6	E7	E 8	E9	E10	N1	N2	N3	N4	N5	N6	N7	N8	N9	N10	A1	A2	A3	A 4	A5
3	53	1	1	1	1	US	4	2	5	2	5	1	4	3	5	1	1	5	2	5	1	1	1	1	1	1	1	5	1	5	2
13	46	1	2	1	1	US	2	2	3	3	3	3	1	5	1	5	2	3	4	2	3	4	3	2	2	4	1	3	3	4	4
1	14	2	2	1	1	PK	5	1	1	4	5	1	1	5	5	1	5	1	5	5	5	5	5	5	5	5	5	1	5	5	1
3	19	2	2	1	1	RO	2	5	2	4	3	4	3	4	4	5	5	4	4	2	4	5	5	5	4	5	2	5	4	4	3
11	25	2	2	1	2	US	3	1	3	3	3	1	3	1	3	5	3	3	3	4	3	3	3	3	3	4	5	5	3	5	1
13	31	1	2	1	2	US	1	5	2	4	1	3	2	4	1	5	1	5	4	5	1	4	4	1	5	2	2	2	3	4	3
5	20	1	2	1	5	US	5	1	5	1	5	1	5	4	4	1	2	4	2	4	2	2	3	2	2	2	5	5	1	5	1
4	23	2	1	1	2	IN	4	3	5	3	5	1	4	3	4	3	1	4	4	4	1	1	1	1	1	1	2	5	1	4	3
5	39	1	2	3	4	US	3	1	5	1	5	1	5	2	5	3	2	4	5	3	3	5	5	4	3	3	1	5	1	5	1
3	18	1	2	1	5	US	1	4	2	5	2	4	1	4	1	5	5	2	5	2	3	4	3	2	3	4	2	3	1	4	2
3	17	2	2	1	1	IT	1	5	2	5	1	4	1	4	1	5	5	3	5	3	2	5	3	3	4	3	2	4	2	4	1
13	15	2	1	1	1	IN	3	3	5	3	3	3	2	4	3	3	1	5	3	3	2	3	2	3	2	4	4	4	2	2	Ę
13	22	1	2	1	2	US	3	3	4	2	4	2	2	3	4	3	3	3	3	3	2	2	4	4	2	3	1	4	1	5	1
3	21	1	2	1	5	US	1	3	2	5	1	1	1	5	1	5	5	3	5	2	5	5	3	2	5	3	1	1	1	4	2
3	28	2	2	1	2	US	3	3	3	4	3	2	2	4	3	5	2	4	4	4	4	4	2	2	3	2	1	4	2	4	2
3	21	1	1	1	5	US	2	3	2	3	3	1	1	3	4	4	2	4	2	4	1	2	2	2	2	2	4	2	4	2	E
13	19	1	2	1	2	FR	1	3	2	4	2	4	1	4	3	4	4	2	3	2	1	3	1	2	2	3	4	2	3	1	4
3	21	1	2	1	5	US	4	1	5	2	5	1	5	3	5	1	5	2	5	2	3	3	3	3	4	2	1	5	2	5	2
3	26	1	2	3	5	GB	2	3	4	3	1	4	1	4	1	5	4	2	5	2	1	4	2	2	2	2	2	2	2	2	2
3	26	1	2	1	1	US	2	2	3	3	3	3	1	3	3	3	4	4	3	1	3	2	2	2	4	4	1	3	2	4	3
40	10	0	0	4	-	1.7	4	4	0	-	0	4	0	4	0	0	4	4	4	4	4	4	_	_	4	0	4	-	4	_	· ·

Learning Hidden Variables & Their Relations

i.i.d. data?	Parametric constraints?	Latent confounders?					
Yes	No	No					
No	Yes	Yes					

• <u>Measured</u> variables (e.g., answer scores in psychometric questionnaires) were <u>generated by causally related latent variables</u>

X1	X2	Х3	X4	X5	X6	X7	X8
4.2	3.6	6.5	6.8	9.6	7.6	2.7	4.8
3.8	1.9	6.5	7.3	8.9	6.9	1.1	4.6
4.2	3.4	6.5	6.9	9.5	7.4	2.5	4.6
4.2	2.2	6.2	6.9	9.6	7.2	1.9	4.8
3.9	1.9	6.5	6.8	9.0	6.8	1.7	4.4
4.0	2.0	6.4	7.2	9.1	7.0	1.0	4.6
3.8	1.7	6.4	7.3	9.0	6.7	0.8	4.3
4.1	2.8	6.5	6.9	9.3	6.7	2.7	4.6



- Find latent variables L_i and their causal relations?
- Rank deficiency or GIN helps solve the problem

Outline

- Why causal/disentangled representations ?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Identifying Latent Causal Model in Linear-Gaussian Cases

Biwei Huang





Motivation

Causal discovery:

- Aims to find causal relationships from observational data, without doing interventions
- Traditionally, assumes no latent confounders and only considers causal structure among observed variables
- However, in some cases, measured variables may not be causal variables, e.g., variables with measurement error, image pixels



Identifying Latent Causal Graphs

Questions to answer:

- Locate (hierarchical) latent variables (i.e., cluster the lower-level variables)
- Identify the causal structure among all variables





X_i: measured variables L_i: latent variables

Motivation of Latent Variable Discovery in AI/ Scientific Discovery

- Usually not possible to measure all task-related variables
 - Causal discovery in the presence of latent variables
 - Image/Video/Language understanding
 - Automatically identify and hierarchically cluster the underlying functional brain areas and discover the information flow, from measured voxel data
 - Identify gene regulation process from gene expression data







An illustration of Tetrad Conditions

Dep₁



 ρ_{ij} denotes the correlation coefficient between x_i and x_j

Applications of Tetrad Conditions

- One-factor measurement model [Silva et al., 2006, Kummerfeld et al., 2016]
- Tree structure [Pearl, 1988, Choi et al., 2011]

One-factor measurement model





Identifying more general latent structures:

LATENT HIERARCHICAL CAUSAL STRUCTURE DISCOVERY WITH RANK CONSTRAINTS

Biwei Huang *1 Charles Low *1, Feng Xie³, Clark Glymour¹, Kun Zhang^{1,2} ¹ Carnegie Mellon University ² Mohamed bin Zayed University of Artificial Intelligence ³ Beijing Technology and Business University, China {bwei.huang, charleslow88, xiefeng009}@gmail.com, cg09@andrew.cmu.edu, kunz1@cmu.edu

Abstract

Most causal discovery procedures assume that there are no latent confounders in the system, which is often violated in real-world problems. In this paper, we consider a challenging scenario for causal structure identification, where some variables are latent and they form a hierarchical graph structure to generate the measured variables; the children of latent variables may still be latent and only leaf nodes are measured, and moreover, there can be multiple paths between every pair of variables (i.e., it is beyond tree structure). We propose an estimation procedure that can efficiently locate latent variables, determine their cardinalities, and identify the latent hierarchical structure, by leveraging rank deficiency constraints over the measured variables. We show that the proposed algorithm can find the correct Markov equivalence class of the whole graph asymptotically under proper restrictions on the graph structure.



SEM with linear causal relations: $X_{i} = \sum_{L_{j} \in Pa(X_{i})} b_{ij}L_{j} + \varepsilon_{X_{i}},$ $L_{j} = \sum_{L_{k} \in Pa(L_{j})} c_{jk}L_{k} + \varepsilon_{L_{j}}$ X_i: measured variables

L_i: latent variables

Questions to answer:

- Locate (hierarchical) latent variables (i.e., cluster the lowerlevel variables)
- Identify the causal structure among latent variables

Basic idea:

- Rank-deficiency constraints over measured variables
 + Specific search procedure foundation of this method
 - $rank(\Sigma_{X_A,X_B})$, which is deficient, indicates the smallest number of variables that t-separate X_A from X_B



Exp: Let $X_A = \{X_{10}, X_{11}\}$ and $X_B = \mathbf{X} \setminus X_A$ rank $(\Sigma_{X_A, X_B}) = 1$ which is rank deficient, because L_6 d-separates X_A from X_B .

However, we cannot directly know the location of these latent variables in the graph

Search procedure:

Input : Date from a set of measured variables X_G Output : Markov equivalence class G'

1. Find clusters and assign latent covers greedily

 $\mathcal{G}' = \mathrm{findCausalClusters} \left(\mathbf{X}_\mathcal{G} \right) \, ;$

2. Refine incorrect clusters and covers from greedy search

 $\mathcal{G}' = ext{refineClusters} (\mathcal{G}');$

3. Refine edges and find v structures

 $\mathcal{G}' = ext{refineEdges} \ (\mathcal{G}') \ ;$

Search procedure:

Input : Date from a set of measured variables X_G Output : Markov equivalence class G'

1. Find clusters and assign latent covers greedily

 $\mathcal{G}' = \mathrm{findCausalClusters} (\mathbf{X}_\mathcal{G}) ;$

2. Refine incorrect clusters and covers from greedy search

 $\mathcal{G}' = ext{refineClusters} (\mathcal{G}');$

3. Refine edges and find v structures

 $\mathcal{G}' = ext{refineEdges} \ (\mathcal{G}') \ ;$

Search procedure:

 I. Find clusters and assign latent covers greedily

 (findCausalClusters)

Rule 1:

If **A** is a rank-deficiency set with rank $(\Sigma_{\mathbf{X}_A,\mathbf{X}_B}) = k$, assign a latent variable **L** with size k as the parents of each A_i



 X_{11}

 X_4

 X_1

 X_8

 X_7

 X_5

Input the data from measured variables

20

Search procedure:

1. Find clusters and assign latent covers greedily *(findCausalClusters)*

X_{8} X_{7} L_{7} L_{7} L_{3} L_{1} L_{2} L_{4} X_{2} X_{11} X_{10} X_{9} X_{1}

Rule 1:

If **A** is a rank-deficiency set with rank $(\Sigma_{\mathbf{X}_A,\mathbf{X}_B}) = k$, assign a latent variable **L** with size k as the parents of each A_i



Exp: Let $\mathbf{X}_A = \{X_5, X_6, X_7\}$ and $\mathbf{X}_B = \mathbf{X} \setminus \mathbf{X}_A$. rank $(\Sigma_{\mathbf{X}_A, \mathbf{X}_B}) = 2$ being rank deficient. Add a latent cover $\{L'_6, L'_7\}$ with size 2 above \mathbf{X}_A .

Search procedure:

 I. Find clusters and assign latent covers greedily

 (findCausalClusters)

Rule 1:

If **A** is a rank-deficiency set with rank $(\Sigma_{\mathbf{X}_A,\mathbf{X}_B}) = k$, assign a latent variable **L** with size k as the parents of each A_i



 X_{11}

 X_4

 X_8

 X_5

Find a latent cover $\{L'_2\}$.

Let $\mathbf{A} = \{L'_4, L'_5\}$. Use its measured descendants $\mathbf{X}_A = \{X_1, X_2, X_3, X_4\}$ as a surrogate for rank test. rank $(\Sigma_{\mathbf{X}_A, \mathbf{X}_B}) = 1$ being rank deficient. Add a latent cover $\{L'_2\}$ with size 1 above \mathbf{A} .

Search procedure:

 I. Find clusters and assign latent covers greedily

 (findCausalClusters)

Rule 1:

If **A** is a rank-deficiency set with rank $(\Sigma_{\mathbf{X}_A,\mathbf{X}_B}) = k$, assign a latent variable **L** with size k as the parents of each A_i



 X_{11}

 X_4

 X_8

 X_5

Use its measured descendants $\mathbf{X}_A = \{X_5, X_6, X_7, X_8\}$ as a surrogate for rank test. rank $(\Sigma_{\mathbf{X}_A, \mathbf{X}_B}) = 1$ being rank deficient. Add a latent cover $\{L'_3\}$ with size 1 above **A**.

Search procedure:

I. Find clusters and assign latent covers greedily *(findCausalClusters)*

Rule 1:

If **A** is a rank-deficiency set with rank $(\Sigma_{\mathbf{X}_A,\mathbf{X}_B}) = k$, assign a latent variable **L** with size k as the parents of each A_i



 X_{11}

 X_4

 X_8

Connect $\{L'_8, L'_9\}$ to $\{L'_2\}$ and to $\{L'_3\}$, and Step 1 ends.

Search procedure:

Input : Date from a set of measured variables X_G Output : Markov equivalence class G'

1. Find clusters and assign latent covers greedily

 $\mathcal{G}' = \mathrm{findCausalClusters} (\mathbf{X}_\mathcal{G}) ;$

2. Refine incorrect clusters and covers from greedy search

 $\mathcal{G}' = ext{refineClusters} (\mathcal{G}');$

3. Refine edges and find v structures

 $\mathcal{G}' = ext{refineEdges} \ (\mathcal{G}') \ ;$

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)





Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters

Pink area: incorrect clusters due to the greedy search in step 1

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)





Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters Refine $\{L'_2\}$ by first removing $\{L'_2\}$ and its parents $\{L'_8, L'_9\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)





Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters Perform *findCausalClusters* over $\{L'_3, L'_4, L'_5, X_9, X_{10}, X_{11}\}$, and then we can find a latent cover $\{L'_{10}\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters

Next perform *findCausalClusters* over $\{L'_{10}, L'_4, L'_5, X_9, X_{10}\}$, and we can find a latent cover $\{L'_{11}\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters Next perform *findCausalClusters* over $\{L'_{11}, L'_4, L'_5, X_9\}$, and we can find a latent cover L'_{12} .

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters Connect $\{L'_{12}\}$ to $\{L'_4, L'_5\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters

Refine $\{L'_3\}$ by first removing $\{L'_3\}$ and its parents $\{L'_{10}\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters Perform *findCausalClusters* over $\{L'_6, L'_7, L'_{11}, X_{11}\}$, and then we can find a latent cover $\{L'_{13}\}$.

Search procedure:

2. Refine incorrect clusters and covers from greedy search (*refineClusters*)



Rule 2:

For each discovered latent cover \mathbf{L} , let $\mathbf{V} = Gp_{G'}(\mathbf{L}) \cup Sib_{G'}(\mathbf{L}) \cup Ch_{G'}(\mathbf{L})$ and apply findCausalClusters to \mathbf{V} to refine the clusters

Connect $\{L'_{13}\}$ to $\{L'_6, L'_7\}$.

Search procedure:

Input : Date from a set of measured variables X_G Output : Markov equivalence class G'

1. Find clusters and assign latent covers greedily

 $\mathcal{G}' = \mathrm{findCausalClusters} \ (\mathbf{X}_\mathcal{G}) \ ;$

2. Refine incorrect clusters and covers from greedy search

 $\mathcal{G}' = ext{refineClusters} (\mathcal{G}');$

3. Refine edges and find v structures

 $\mathcal{G}' = ext{refineEdges} \ (\mathcal{G}') \ ;$

Search procedure:



3. Refine edges and find v structures *(refineEdges)*

Rule 3:

For a pair $(\mathbf{L}_A, \mathbf{L}_B)$, let $\mathcal{A} \leftarrow {\mathbf{L}_A, \mathbf{C}_1^A, \mathbf{C}_2^A, ...}$ and $\mathcal{B} \leftarrow {\mathbf{L}_B, \mathbf{C}_1^B, \mathbf{C}_2^B, ...}$.

If there exists such \mathcal{A}, \mathcal{B} such that $\operatorname{rank}_{\mathcal{G}'}(\Sigma_{\mathcal{A},\mathcal{B}})$ is rank deficient, remove all edges between $\mathbf{L}_A, \mathbf{L}_B$ in \mathcal{G}'



Perform *refineEdges* to refine the edges and output the Markov equivalence class.

Search procedure:

3. Refine edges and find v structures *(refineEdges)*

Another example that contains the v structure:



Possible Output from Phase II.



A graph with v structure.
Search procedure:

3. Refine edges and find v structures *(refineEdges)*

Another example that contains the v structure:



Possible Output from Phase II.



Connect L'_2 and L'_3



A graph with v structure.

Search procedure:

3. Refine edges and find v structures *(refineEdges)*

Another example that contains the v structure:



Possible Output from Phase II.





A graph with v structure.

Remove the edge between L'_2 and L'_3

Let $\mathcal{A} = \{L'_2, X_1\}$ and $\mathcal{B} = \{L'_3, X_2\}$ rank $(\Sigma_{\mathcal{A},\mathcal{B}}) = 1$ being rank deficient It means that L'_1 d-separates L'_2 from L'_3 Remove the edge between L'_2 and L'_3

Search procedure:

3. Refine edges and find v structures *(refineEdges)*

Another example that contains the v structure:



Possible Output from Phase II.





A graph with v structure.

Form a V structure: $L'_2 \rightarrow L'_4 \leftarrow L'_3$.

Let
$$\mathcal{A}^1 = \{L'_2, L'_4, X_1\}$$
 and $\mathcal{B}^1 = \{L'_3, X_2\}$
rank $(\Sigma_{\mathcal{A}^1, \mathcal{B}^1}) = 2 > 1 = \operatorname{rank}(\Sigma_{\mathcal{A}, \mathcal{B}})$
Let $\mathcal{A}^2 = \{L'_2, X_1\}$ and $\mathcal{B}^2 = \{L'_3, L'_4, X_2\}$
rank $(\Sigma_{\mathcal{A}^2, \mathcal{B}^2}) = 2 > 1 = \operatorname{rank}(\Sigma_{\mathcal{A}, \mathcal{B}})$
so $L'_2 \to L'_4 \leftarrow L'_3$

Main identifiability condition:

For each latent variable set \mathbf{L} with size k, it has

- at least k+1 pure children (can be either latent or measured) and
- another k+1 neighbors

Pure children: if V are pure children of latent variables L, then V do not have other parents besides L



Exp: Let L={L₂,L₃} with size 2: 3 pure children: {L₆,L₇,L₈} 3 neighbors: {L₁,L₉,L₁₀}

The proposed approach works for

- \checkmark Latent hierarchical causal structure with linear causal relations
- ✓ Each latent variable set with size k has at least (k+1) pure children
- \checkmark Multiple latent parents for each (measured or latent) variable

Extension to the general case: to allow observed variables to be causes as well

- Direct causal influences among observed variables
 - In the special case with no latent variables, it returns the same graph as the PC algorithm
- Causal-related latent variables
 - Latent variables may form a hierarchical structure
 - Latent variables can serve as both confounders and intermediate variables for observed variables



Xinshuai Dong, Biwei Huang, Peter Spirtes, Kun Zhang, et al., ongoing work

Extension to the general case: to allow observed variables to be causes as well

Conditional independence Vs. Rank:

let A, B, and C be disjoint subsets of [m]. Then the conditional independence statement $X_A \perp \!\!\!\perp X_B | X_C$ holds for X, if and only if $\Sigma_{A \cup C, B \cup C}$ has rank C.





(b) Take $\mathcal{X} = \{\{X_2, X_3\}\}$ and $\mathcal{C} = \{\{X_7\}, \{X_8\}\}.$

 $rank(\Sigma_{\mathcal{C}\cup\mathcal{X},\mathcal{N}\cup\mathcal{X}})=2$



$$\mathit{rank}(\Sigma_{\mathcal{C}\cup\mathcal{X},\mathcal{N}\cup\mathcal{X}})=2$$



(d) Take $\mathcal{X} = \{\}$ and $\mathcal{C} = \{\{X_1\}, \{L_2, X_2\}, \{X_3\}\}$ $rank(\Sigma_{\mathcal{C}\cup\mathcal{X},\mathcal{N}\cup\mathcal{X}}) = 1$

Extension to the general case: To allow observed variables to be causes as well

		F1 score for skeleton among $\mathbf{X}_{\mathcal{G}}$						
Algorithm		Ours	Hier. rank	PC	FCI	GIN	RCD	
Observed only	2k	0.95 (0.04)	-	0.78 (0.01)	0.07 (0.01)	-	0.79 (0.01)	
	5k	0.97 (0.01)	-	0.81 (0.01)	0.15 (0.07)	-	0.91 (0.01)	
	10k	0.98 (0.02)	-	0.82 (0.01)	0.25 (0.18)	-	0.93 (0.01)	
Latent+tree	2k	0.79 (0.16)	-	0.46 (0.02)	0.00 (0.00)	-	0.30 (0.03)	
	5k	0.86 (0.10)	-	0.44 (0.00)	0.03 (0.04)	-	0.38 (0.01)	
	10k	0.97 (0.04)	-	0.44 (0.00)	0.18 (0.07)	-	0.39 (0.02)	
Latent+measm	2k	0.84 (0.11)	-	0.50 (0.02)	0.00 (0.00)	-	0.30 (0.02)	
	5k	0.93 (0.08)	-	0.49 (0.01)	0.05 (0.03)	-	0.32 (0.02)	
	10k	0.95 (0.05)	-	0.48 (0.02)	0.03 (0.05)	-	0.42 (0.09)	
Latent general	2k	0.68 (0.02)	-	0.44 (0.01)	0.27 (0.09)	-	0.39 (0.06)	
	5k	0.71 (0.03)	-	0.45 (0.01)	0.31 (0.10)	-	0.44 (0.05)	
	10k	0.78 (0.06)	-	0.45 (0.01)	0.32 (0.05)	-	0.44 (0.01)	

		F1 score for skeleton among $V_{\mathcal{G}}$ (both $X_{\mathcal{G}}$ and $L_{\mathcal{G}}$)						
Algorithm		Ours	Hier. rank	PC	FCI	GIN	RCD	
Latent+tree	2k	0.84 (0.11)	0.58 (0.01)	0.36 (0.01)	0.00 (0.00)	0.37 (0.03)	0.24 (0.04)	
	5k	0.92 (0.05)	0.60 (0.01)	0.36 (0.00)	0.02 (0.02)	0.41 (0.03)	0.33 (0.00)	
	10k	0.98 (0.02)	0.60 (0.01)	0.36 (0.00)	0.15 (0.08)	0.41 (0.03)	0.33 (0.01)	
Latent+measm	2k	0.81 (0.12)	0.52 (0.05)	0.37 (0.01)	0.00 (0.00)	0.40 (0.02)	0.26 (0.03)	
	5k	0.88 (0.11)	0.52 (0.05)	0.49 (0.01)	0.04 (0.03)	0.46 (0.03)	0.29 (0.01)	
	10k	0.91 (0.09)	0.53 (0.05)	0.49 (0.01)	0.02 (0.03)	0.47 (0.05)	0.34 (0.04)	
Latent general	2k	0.66 (0.01)	0.44 (0.02)	0.31 (0.01)	0.17 (0.06)	0.30 (0.04)	0.32 (0.03)	
	5k	0.72 (0.03)	0.45 (0.03)	0.33 (0.01)	0.21 (0.07)	0.38 (0.04)	0.34 (0.02)	
	10k	0.80 (0.05)	0.45 (0.04)	0.33 (0.01)	0.21 (0.04)	0.35 (0.01)	0.36 (0.01)	

Example: Big 5 Questions Are Well Designed but...

Big 5:

openness; conscientiousness; extraversion; agreeableness; neuroticism



Intermediate Summary: Identifying Latent Causal Graphs

- Further issues...
 - Weaker conditions on the structure?
 - Nonstationary cases?
 - More general or domain-specific cases?





X_i: measured variables L_i: latent variables

Outline

- Why?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Recap: Independent Noise (IN) Condition

 $Z \longrightarrow Y$

- (**Z**, *Y*) follows the <u>IN condition</u> iff regression residual $Y \tilde{w}^{\intercal} \mathbf{Z}$ is independent from **Z**
- Help determine causal orders and estimate the Linear, Non-Gaussian Acyclic Causal model (LiNGAM)





 $= cE_2 - bE_3,$

independent from L_1 and from X_1 ,

and we know $\frac{b}{c} = \frac{Cov(X_2, X_3)}{Cov(X_1, X_3)}$

Nontrivial linear combination of X_2 and X_3 will involve the noise term in L_1 , hence dependent on X_1

Linear, Non-Gaussian Case: GIN

• Generalized Independent Noise (GIN) Condition: (Z, Y) follows the GIN condition $\iff \omega^{\top} Y \perp Z$, where $\omega^{\top} \text{Cov}(Y, Z) = 0$ and $\omega \neq 0$

• Graphical criterion

(Z, Y) follows the GIN condition iff there is an exogenous set S of PA(Y) that blocks all paths between Y and Z, where 0<=|S|<=min(|Z|, |Y|-1)



X_i: observed variables L_i: latent variables

GIN Condition for Estimating Linear Non-Gaussian Latent Graphs

- A two-step algorithm to identify the latent variable graph
 - By testing for GIN conditions over the input X_1, \dots, X_8



Step 2: determine *causal structure* of the latent variables



GIN-Based Method: Application to Teacher's Burnout Data

- Contains 28 measured variables
- Discovered clusters and causal order of the latent variables:

Causal Clusters	Observed variables
$\mathcal{S}_{1}\left(1 ight)$	$RC_1, RC_2, WO_1, WO_2,$
	DM_1, DM_2
$\mathcal{S}_{2}\left(1 ight)$	CC_1, CC_2, CC_3, CC_4
$\mathcal{S}_{3}\left(1 ight)$	PS_1, PS_2
$\mathcal{S}_{4}\left(1 ight)$	$ELC_1, ELC_2, ELC_3, ELC_4,$
	ELC_5
$\mathcal{S}_{5}(2)$	$SE_1, SE_2, SE_3, EE_1,$
	EE_2, EE_3, DP_1, PA_3
$\mathcal{S}_{6}(3)$	DP_2, PA_1, PA_2

 $L(S_1) > L(S_2) > L(S_3) > L(S_5) > L(S_4) > L(S_6).$ (from root to leaf)

• Consistent with the hypothesized model





- Xie, Cai, Huang, Glymour, Hao, Zhang, "Generalized Independent Noise Condition for Estimating Linear Non-Gaussian Latent Variable Causal Graphs," NeurIPS 2020
- Cai, Xie, Glymour, Hao, Zhang, "Triad Constraints for Learning Causal Structure of Latent Variables," NeurIPS 2019

Outline

- Why?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Identifiability of nonlinear ICA: challenge

Is nonlinear ICA identifiable?











Identifiability of nonlinear ICA: auxiliary variables



[Hyvarinen et al., Nonlinear ICA Using Auxiliary Variables and Generalized Contrastive Learning, AISTAT 2019]

Identifiability of nonlinear ICA: structural sparsity

(Structural Sparsity) For all $k \in \{1, ..., n\}$, there exists C_k such that

$$\bigcap_{i \in \mathcal{C}_k} \operatorname{supp}(\mathbf{J}_{\mathbf{f}}(\mathbf{s})_{i,:}) = \{k\}.$$





Graphically, for every latent source **s_i**, there exists a set of observed variable(s) such that the intersection of their/its parent(s) is **s_i**

Example: for **s_1**, there exists **x_1** and **x_4** such that the intersection of their parents is **s_1**

Failure: two sources influence the same set of observed variables

[Zheng et al., On the Identifiability of Nonlinear ICA: Sparsity and Beyond, NeurIPS 2022]

Identifiability of nonlinear ICA: real-world images

Line thickness

Angle

Upper width

Height



Identification results on EMNIST

Each row represents an identified source with its value varying

Outline

- Why?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Nonlinear ICA with Multiple Domains

i.i.d. data?	Parametric constraints?	Latent confounders?		
Yes	No	No		
No	Yes	Yes		

- Nonlinear ICA: observed variables follow $\mathbf{X} = \mathbf{g}(\mathbf{Z})$, in which Z_i are mutually independent
 - Solutions to nonlinear ICA high non-unique
 - If the dstr of each Z_i change across multiple domains, generally their are identifiable (up to component-wise transformations)

• Why?
$$\theta_1 \longrightarrow Z_1 \xrightarrow{Z_1} g \xrightarrow{X_1} for \mathbf{Z}' = h(\mathbf{Z}): \theta_1 \xrightarrow{Z'_1} g' \xrightarrow{X_1} X_2$$

- Hyvärinen, Pajunen, Nonlinear independent component analysis: Existence and uniqueness results. Neural networks, 1999.
- Hyvarinen, Sasaki, Turner, "Nonlinear ICA using auxiliary variables and generalized contrastive learning," In The 22nd International Conference on Artificial Intelligence and Statistics, 2019.

Partial Identifiability for Domain Adaptation

Lingjing Kong¹ Shaoan Xie¹ Weiran Yao¹ Yujia Zheng¹ Guangyi Chen²¹ Petar Stojanov³ Victor Akinwande¹ Kun Zhang²¹

Abstract

Unsupervised domain adaptation is critical to many real-world applications where label information is unavailable in the target domain. In general, without further assumptions, the joint distribution of the features and the label is not identifiable in the target domain. To address this issue, we rely on a property of minimal changes of causal mechanisms across domains to minimize unnecessary influences of domain shift. To encode this property, we first formulate the data generating process using a latent variable model with two partitioned latent subspaces: invariant components whose distributions stay the same across domains, and sparse changing components that vary across domains. We further constrain the domain shift to have a restrictive influence on the changing components. Under mild conditions, we show that the latent variables are partially identifiable, from

domain indices u, the training (source domain) data follows multiple joint distributions $p_{\mathbf{x},\mathbf{y}|\mathbf{u}_1}$, $p_{\mathbf{x},\mathbf{y}|\mathbf{u}_2}$, ..., $p_{\mathbf{x},\mathbf{y}|\mathbf{u}_M}$,¹ and the test (target domain) data follows the joint distribution $p_{\mathbf{x},\mathbf{y}|\mathbf{u}^{T}}$, where $p_{\mathbf{x},\mathbf{y}|\mathbf{u}}$ may vary across \mathbf{u}_1 , \mathbf{u}_2 , ..., \mathbf{u}_M . During training, for each *i*-th source domain, we are given labeled observations $(\mathbf{x}_k^{(i)}, \mathbf{y}_k^{(i)})_{k=1}^{m_i}$ from $p_{\mathbf{x},\mathbf{y}|\mathbf{u}_i}$, and target domain unlabeled instances $(\mathbf{x}_k^T)_{k=1}^{m_T}$ from $p_{\mathbf{x},\mathbf{y}|\mathbf{u}^{T}}$. The main goal of domain adaptation is to make use of the available observed information, to construct a predictor that will have optimal performance in the target domain.

It is apparent that without further assumptions, this objective is ill-posed. Namely, since the only available observations in the target domain are from the marginal distribution $p_{\mathbf{x}|\mathbf{u}^{\mathcal{T}}}$, the data may correspond to infinitely many joint distributions $p_{\mathbf{x},\mathbf{y}|\mathbf{u}^{\mathcal{T}}}$. This mandates making additional assumptions on the relationship between the source and the target domain distributions, with the hope to be able to reconstruct (identify) the joint distribution in the target domain $p_{\mathbf{x},\mathbf{y}|\mathbf{u}^{\mathcal{T}}}$. Typically, these assumptions entail some measure of sim-

Finding Changing Hidden Variables for Transfer Learning

i.i.d. data?	Parametric constraints?	Latent confounders?		
Yes	No	No		
No	Yes	Yes		



- Underlying components Z_S may change across domains
- Changing components Z_S are identifiable; invariant part Z_C are identifiable up to its subspace
- Using invariant part \mathbf{Z}_{C} and transformed changing part $\tilde{\mathbf{Z}}_{S}$ for prediction

Models	$\rightarrow \operatorname{Art}$	\rightarrow Clipart	\rightarrow Product	\rightarrow Realworld	Avg
Source Only (He et al., 2016)	64.58 ± 0.68	52.32 ± 0.63	77.63 ± 0.23	$80.70 {\pm} 0.81$	68.81
DANN (Ganin et al., 2016)	64.26±0.59	$58.01 {\pm} 1.55$	$76.44 {\pm} 0.47$	$78.80{\pm}0.49$	69.38
DANN+BSP (Chen et al., 2019)	66.10±0.27	$61.03 {\pm} 0.39$	$78.13 {\pm} 0.31$	$79.92{\pm}0.13$	71.29
DAN (Long et al., 2015)	68.28±0.45	$57.92 {\pm} 0.65$	$78.45{\pm}0.05$	$81.93 {\pm} 0.35$	71.64
MCD (Saito et al., 2018)	$67.84{\pm}0.38$	$59.91 {\pm} 0.55$	$79.21 {\pm} 0.61$	$80.93 {\pm} 0.18$	71.97
M3SDA (Peng et al., 2019)	66.22±0.52	$58.55 {\pm} 0.62$	$79.45 {\pm} 0.52$	81.35±0.19	71.39
DCTN (Xu et al., 2018)	66.92 ± 0.60	$61.82{\pm}0.46$	$79.20 {\pm} 0.58$	$77.78 {\pm} 0.59$	71.43
MIAN (Park & Lee, 2021)	69.39±0.50	$63.05 {\pm} 0.61$	$79.62 {\pm} 0.16$	$80.44 {\pm} 0.24$	73.12
MIAN- γ (Park & Lee, 2021)	69.88±0.35	$64.20{\pm}0.68$	$80.87 {\pm} 0.37$	$81.49 {\pm} 0.24$	74.11
iMSDA (Ours)	75.77±0.21	$60.83 {\pm} 0.73$	84.13±0.09	$84.83{\pm}0.12$	76.39

Table 2. Classification results on Office-Home. Backbone: Resnet-50. Baseline results are taken from (Park & Lee, 2021).

- Kong, Xie, Yao, Zheng, Chen, Stojanov, Akinwande, Zhang, Partial disentanglement for domain adaptation, ICML 2022

Unsupervised Image-to-Image Translation





Images from the winter season domain.

MULTI-DOMAIN IMAGE GENERATION AND TRANSLA-TION WITH IDENTIFIABILITY GUARANTEES

Shaoan Xie¹, Lingjing Kong¹, Mingming Gong^{3,2}, and Kun Zhang^{1,2}

¹ Carnegie Mellon University ²Mohamed bin Zayed University of Artificial Intelligence ³The University of Melbourne shaoan@cmu.edu, lingjingkong@cmu.edu, mingming.gong@unimelb.edu.au, kunz1@cmu.edu

ABSTRACT

Multi-domain image generation and unpaired image-to-to-image translation are two important and related computer vision problems. The common technique for the two tasks is the learning of a joint distribution from multiple marginal distributions. However, it is well known that there can be infinitely many joint distributions that can derive the same marginals. Hence, it is necessary to formulate suitable constraints to address this highly ill-posed problem. Inspired by the recent advances in nonlinear Independent Component Analysis (ICA) theory, we propose a new method to learn the joint distribution from the marginals by enforcing a specific type of minimal change across domains. We report one of the first results connecting multi-domain generative models to identifiability and shows

Sample Images Generated by Generative Adversarial Networks (GANs)



Images generated by a **GAN created by NVIDIA**.

GANs



Minimax game which G wants to minimize V while D wants to maximize it: $\min_{G} \max_{D} V(D,G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))].$



- Match the data distribution across domains, while the dimensionality of $\epsilon_S^{(u)}$ is as small as possible (minimal changes across domains **controlled by** λ ; no penalty when λ =0)
- Correspondence relations among domains are identifiable

Multi-domain Image Generation & Translation with Identifiability Guarantees

- Idea: Matching the distributions across domains with a minimal number of changing components
- Correspondence info (joint distribution) identifiable under mild assumptions
- Example: Generating female & males images with the same "content"

Ours ($\chi = 0.1$)

StyleGAN2-ADA

TGAN



- Xie, Kong, Gong, Zhang, "Multi-domain image generation and translation with identifiability guarantees", ICLR 2023

More results...



Figure 10: CelebA-HQ. Without the sparsity regularization, i.e., $\lambda = 0$, we observe some unnecessary changes between the image tuples in each row. For example, e.g., the added sun-glasses and skin color change in the first row. TGAN changes the background (first row of third panel). CoGAN changes the skin color (second row, second panel).

More results...



Figure 11: AFHQ. StyleGAN2-ADA changes animal poses in many examples, e.g., second and third row of first panel. Our base ($\lambda = 0$) also changes the poses, e.g., first and third row of second panel. CoGAN and TGAN are slightly better in preserving poses but we can observe that some generated images are unrealistic. For example, the wolf (first row, third panel of TGAN) and the dog (third row, third panel of CoGAN).

Outline

- Why?
- How?
 - IID case
 - Linear-Gaussian case
 - Linear, non-Gaussian case
 - Nonlinear case
 - From multiple distributions
 - With temporal information

Temporally Disentangled Representation Learning

Weiran Yao CMU weiran@cmu.edu

Guangyi Chen CMU & MBZUAI guangyichen1994@gmail.com Kun Zhang CMU & MBZUAI kunz1@cmu.edu

Abstract

Recently in the field of unsupervised representation learning, strong identifiability results for disentanglement of causally-related latent variables have been established by exploiting certain side information, such as class labels, in addition to independence. However, most existing work is constrained by functional form assumptions such as independent sources or further with linear transitions, and distribution assumptions such as stationary, exponential family distribution. It is unknown whether the underlying latent variables and their causal relations are identifiable if they have arbitrary, nonparametric causal influences in between. In this work, we establish the identifiability theories of nonparametric latent causal processes from their nonlinear mixtures under fixed temporal causal influences and analyze how distribution changes can further benefit the disentanglement. We propose TDRL a principled framework to recover time-delayed latent causal vari-

Learning Latent Causal Dynamics



- Yao, Chen, Zhang, "Causal Disentanglement for Time Series," NeurIPS 2022
- Yao, Sun, Ho, Sun, Zhang, "Learning Temporally causal latent processes from general temporal data," ICLR 2022
Comparisons

i.i.d. data?	Parametric constraints?	Latent confounders?	Learn the underlying causal dynamics from
Yes	No	No	<i>"Time-delayed" influence</i> renders latent processes
No	Yes	Yes	& their relations identifiable

Table 1: Attributes of nonlinear ICA theories for time-series. A check denotes that a method has an attribute or can be applied to a setting, whereas a cross denotes the opposite. [†] indicates our approach.

Theory	Time-varying Relation	Causally-related Process	Partitioned Subspace	Nonparametric Transition	Applicable to Stationary Environment
PCL	×	X	×	✓	 ✓
GCL	✓	X	×	\checkmark	1
HM-NLICA	×	X	×	×	×
SlowVAE	×	X	×	×	1
SNICA	✓	\checkmark	×	×	×
i-VAE	✓	X	×	×	×
LEAP	X	\checkmark	×	\checkmark	X
TDRL †	1	✓	1	1	✓

- Yao, Chen, Zhang, "Causal Disentanglement for Time Series," NeurIPS 2022

- Yao, Sun, Ho, Sun, Zhang, "Learning Temporally causal latent processes from general temporal data," ICLR 2022

Results on Video Data

• For easy interpretation, consider two simple video data sets

- KiTTiMask: a video dataset of binary pedestrian masks
- Mass-spring system: a video dataset with ball movement and invisible springs



- Yao, Chen, Zhang, "Learning Latent Causal Dynamics," NeurIPS 2022

- Yao, Sun, Ho, Sun, Zhang, "Learning Temporally causal latent processes from general temporal data," ICLR 2022

Causal Representation Learning: A Summary

i.i.d. data?	Parametric constraints?	Latent confounders?	What can we get?	
	NLa	No	(Different types of) equivalence class	
Vee	INO	Yes		
res	Vee	No	Unique identifiability (under structural conditions)	
	res	Yes		
	No/Yes	No	(Extended) regression	
NON-I, DULI.D.		Yes	Latent temporal causal processes identifiable!	
	No	Nia	More informative than MEC (CD-NOD)	
	Yes	INO	May have unique identifiability	
I., DUL HOH-I.D.	No	Vee	Changing subspace identifiable	
	Yes	Tes	Variables in changing relations identifiable	

Summary

- Essential to learn hidden causal variables in many cases!
- Possible to achieve even in the IID case
- Benefit from distribution changes and temporal information
- Future work
 - Efficient procedure?
 - Necessary and sufficient identifiability conditions?
 - Changing relations among hidden variables?