Reasoning about Independence in Probabilistic Models of Relational Data

Marc Maier, Katerina Marazopoulou, David Jensen

A Sound and Complete Algorithm for Learning Causal Models from Relational Data

Marc Maier, Katerina Marazopoulou, David Arbour, David Jensen

Knowledge Discovery Laboratory • University of Massachusetts Amherst



The "world"



Bayesian network

[Pearl 1988]

The "world"



Bayesian network

[Verma & Pearl 1988; Geiger & Pearl 1988]

conditional independencies 0 d-separation produces { **o** } The "world" 0

Bayesian network

[Verma & Pearl 1988; Geiger & Pearl 1988]





[Pearl 2000; Spirtes et al. 2000]





[Maier et al. 2013]





[Maier et al. 2013]

Topics

Background on relational data and models

Relational *d*-separation

The RCD algorithm

Ground graph



Ground graph



Instance independence

Mode

The variables on any data instance are *marginally independent* of all variables on every other data instance

Employee *n*

Ground graph



Ground graph



Identically distributed

The same variable on every data instance is drawn from the same underlying conditional distribution

Employee

Mode

Employee *n*

Ground graph



Ground graph

Employee 1



Employee n

Relational models and non-i.i.d. data

Ground graph



Focus on directed graphical models of relational data to represent causal dependencies (e.g., PRMs, DAPER models, plate models).

[Getoor, Friedman, Koller, Pfeffer & Taskar 2007; Heckerman, Meek & Koller 2007; Buntine 1994; Gilks, Thomas & Spiegelhalter et al. 1994]

Examples of relational data

- Scholarly publishing
 - Researchers, articles, citations, venues
- Epidemiology
 - Individuals, contagions, treatments, interactions
- Sports
 - Athletes, teams, coaches, referees, competitive interactions
- Neuroscience
 - Molecular, cellular, system, cognitive levels
- Movie industry
 - Movies, actors, directors, studios, critic reviews
- Organizations
 - Employees, products, business units

Relational models generalize other classes of models

- Bayesian networks
 [Pearl 2000; Spirtes et al. 2000]
- Models of interference / spillover effects / violations of SUTVA

[Rosenbaum 2007; Hudgens & Halloran 2008; Manski 2010; Tchetgen Tchetgen & VanderWeele 2012]

- Models of networks
 (e.g., p1, p*, ERGMs)
 [Holland & Leinhardt 1981; Snijders 2002; Robins et al. 2007]
- Multilevel / hierarchical / random











Overview of template models add dependencies Schema — Model ntiate add dependencies instantiate Skeleton ---- Ground graph instantiate instantiate

Bayesian networks as template models



Relational models as template models



- Expected types of items
- Expected attributes
- How often entities can participate in relationships



- Expected types of items
- Expected attributes
- How often entities can participate in relationships



- Expected types of items
- Expected attributes
- How often entities can participate in relationships



- Expected types of items
- Expected attributes
- How often entities can participate in relationships



Relational skeletons

A relational skeleton is an instantiated relational schema

- Set of entity and relationship instances
- Adheres to cardinality constraints



Relational paths

A relational path is an alternating sequence of entity and relationship classes

- Specifies how to get from one type of item to another
- Building blocks for relational variables
- Length limited by domain-specific, user-defined hop threshold
- Base item on path has the special designation of perspective



[Employee, Develops, Product]

DEVELOPS

PRODUC[®]

EMPLOYE



The set of terminal items reached by a particular base item instance via a relational path on a relational skeleton



```
[Employee]|<sub>Roger</sub> = {Roger}
```

The set of terminal items reached by a particular base item instance via a relational path on a relational skeleton



[Employee, Develops, Product]|_{Roger} = {Laptop}

The set of terminal items reached by a particular base item instance via a relational path on a relational skeleton



[Employee, Develops, Product, Funds, Business-Unit]|_{Roger} = {Devices}

The set of terminal items reached by a particular base item instance via a relational path on a relational skeleton



[Employee, Develops, Product, Develops, Employee]|_{Roger} = {Quinn, Sally}

Relational variables and their terminal sets

Relational variables attach an attribute to a relational path

Building blocks for relational dependencies
 Instantiations are sets of random variable instances for a particular base item instance



[Employee].Competence|_{Roger} = {Roger.Competence}

Relational variables and their terminal sets

Relational variables attach an attribute to a relational path

Building blocks for relational dependencies
 Instantiations are sets of random variable instances for a particular base item instance



[Employee, Develops, Product].Success|_{Roger} = {Laptop.Success}

Relational variables and their terminal sets

Relational variables attach an attribute to a relational path

Building blocks for relational dependencies
 Instantiations are sets of random variable instances for a particular base item instance



[Employee, Develops, Product, Funds, Business-Unit].Revenue|_{Roger} = {Devices.Revenue}
Relational variables and their terminal sets

Relational variables attach an attribute to a relational path

Building blocks for relational dependencies
 Instantiations are sets of random variable instances for a particular base item instance



[Employee, Develops, Product, Develops, Employee].Salary_{|Roger} = {Quinn.Salary, Sally.Salary}

A relational dependency combines a pair of relational variables with a common perspective

- Referred to as treatment/outcome, cause/effect, parent/child
- Canonical form has singleton outcome path
- Building blocks for relational models



A relational dependency combines a pair of relational variables with a common perspective

- Referred to as treatment/outcome, cause/effect, parent/child
- Canonical form has singleton outcome path
- Building blocks for relational models



A relational dependency combines a pair of relational variables with a common perspective

- Referred to as treatment/outcome, cause/effect, parent/child
- Canonical form has singleton outcome path
- Building blocks for relational models



A relational dependency combines a pair of relational variables with a common perspective

- Referred to as treatment/outcome, cause/effect, parent/child
- Canonical form has singleton outcome path
- Building blocks for relational models



A relational dependency combines a pair of relational variables with a common perspective

- Referred to as treatment/outcome, cause/effect, parent/child
- Canonical form has singleton outcome path
- Building blocks for relational models



Ground graphs

A ground graph is an instantiated relational model for a given relational skeleton

- Applies relational dependencies to the variable instances governed by a relational skeleton
- Connects the terminal sets of the parent relational variable to the terminal set of the child relational variable



Ground graphs

A ground graph is an instantiated relational model for a given relational skeleton

- Applies relational dependencies to the variable instances governed by a relational skeleton
- Connects the terminal sets of the parent relational variable to the terminal set of the child relational variable



Ground graphs

A ground graph is an instantiated relational model for a given relational skeleton

- Applies relational dependencies to the variable instances governed by a relational skeleton
- Connects the terminal sets of the parent relational variable to the terminal set of the child relational variable



Probabilistic semantics of ground graphs



- If a ground graph is acyclic, then it has a coherent joint probability distribution
- If a relational model is acyclic, then any ground graph is acyclic [Getoor 2001]

Probabilistic semantics of ground graphs



 $P(\mathcal{V}) = \prod_{v \in \mathcal{V}} P(v \mid parents(v)) \text{ Independent instance}$

 $P(GG_{\mathcal{M}\sigma}) = \prod_{v \in \mathcal{V}} \prod_{i \in \sigma(I)} P(v_i \mid parents(v_i)) \text{ Set of independent instances}$ (ground graph of a Bayesian network)

 $P(GG_{\mathcal{M}\sigma}) = \prod_{I \in \mathcal{E} \cup \mathcal{R}} \prod_{X \in \mathcal{A}(I)} \prod_{i \in \sigma(I)} P(i.X \mid parents(i.X))$ Ground graph of a relational model

Summary of relational concepts **Relational paths** compose relational variables compose relational dependencies compose relational models (all constrained by a **relational schema**), which applied to a relational skeleton produces a ground graph.

Concepts underlie the theory of relational *d*-separation and support the algorithmic details of the relational causal discovery algorithm.

Questions?

Topics

✓ Background on relational data and models

Relational *d*-separation

The RCD algorithm

Why is *d*-separation useful?

- Grounded in theory—Equivalent to global Markov condition
- Algorithmic—Simple set of graphical rules for derivation of conditional independence facts
- Sound and complete—Produces model implications that hold for all possible model instantiations
- Enables constraint-based learning—Algorithms can leverage the connection between causal structure and conditional independence

d-separation and ground graphs



$X \perp Y \mid \{ V \}$ $X \perp W \mid \{ V \}$



 $\begin{array}{c} X_1 \coprod Y_1 \mid \{V_1\} \\ X_1 \coprod W_1 \mid \{V_1\} \end{array}$



 $X_2 \perp \mid Y_2 \mid \{V_2\}$

 $X_2 \downarrow W_2 | \{V_2\}$



 $\begin{array}{c} X_3 \coprod Y_3 \middle| \{V_3\} \\ X_3 \coprod W_3 \middle| \{V_3\} \end{array}$

:



 $Xn \not \downarrow Wn \big| \{V_n\}$











[Employee].*Competence* [Employee, Product, Business-Unit].*Revenue* [{ [Employee, Product].*Success*, [Employee, Product, Employee].*Competence* } Towards a theory of *d*-separation for relational models

- Why not test for *d*-separation at the *model level*?
 - **Relational** *d*-connecting paths that are only manifest in ground graphs.
- Why not test for *d*-separation on *ground graphs*?
 - Impractical to have tests on a representation that scales with sample size (ground graphs can be arbitrarily large).
 - A ground graph is a **single data sample** from all represented skeletons and distributions of a relational model.

Defining relational *d*-separation

Let $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$ be distinct sets of relational variables for perspective $B \in \mathcal{E} \cup \mathcal{R}$ for relational schema \mathcal{S} .

For relational model \mathcal{M} , \mathbf{X} and \mathbf{Y} are *d*-separated by \mathbf{Z} if and only if, for any skeleton σ , $\mathbf{X}|_b$ and $\mathbf{Y}|_b$ are *d*-separated by $\mathbf{Z}|_b$ in ground graph $GG_{\mathcal{M}\sigma}$ for all $b \in \sigma(B)$.

all possible ground graphs all instances

...which suggests we need a representation that **abstracts** over all possible ground graphs.

Defining abstract ground graphs

An abstract ground graph $AGG_{\mathcal{M}Bh} = (V, E)$ for relational model $\mathcal{M} = (\mathcal{S}, \mathcal{D})$, perspective $B \in \mathcal{E} \cup \mathcal{R}$, and hop threshold $h \in \mathbb{N}^0$ abstracts dependencies \mathcal{D} for all possible ground graphs $GG_{\mathcal{M}\sigma}$ of \mathcal{M} for all skeletons σ .

Abstract ground graphs capture all possible paths of dependence with two primary innovations:

- (1) Dependencies are translated across all perspectives
- (2) Intersection variables are explicitly represented for pairs of relational variables that may intersect in some skeleton

Abstract ground graphs abstract ground graphs

- Lifted representation: Lies between the model level and the ground graph level.
- *Data-free*: Constructed with knowledge of only the model structure (*M*), a single perspective (*B*), and a hop threshold (*h*).
- Sound and complete: (1) Every dependency in the abstract ground graph exists in some ground graph and (2) any dependency in any ground graph exists in the abstract ground graph.
- Generalizes Bayesian networks: For schemas with a single entity class, the abstract ground graph is equivalent to the model.

Constructing abstract ground graphs





[Employee, Product, Employee, Product]|_{Roger} = {Case, Adapter, Tablet}



[Employee, Product, Employee, Product]|_{Roger} = {Case, Adapter, Tablet}

[Employee, Product, Business-Unit, Product]|_{Roger} = {Tablet, Smartphone}





= {Tablet}

d-separation on abstract ground graphs

Given a query:

Is X d-separated from Y given Z?

Answer by checking:

Is $\bar{\mathbf{X}}$ *d*-separated from $\bar{\mathbf{Y}}$ given $\bar{\mathbf{Z}}$?

on the abstract ground graph for the common **perspective**, where the **augmented** sets include subsumed intersection variables

- Because abstract ground graphs capture all paths of dependence, it suffices to check if all pairwise elements in $\overline{\mathbf{X}}$ and $\overline{\mathbf{Y}}$ are *d*-separated by $\overline{\mathbf{Z}}$.
- Reflects all dependency paths for any possible variable instance pair in any ground graph represented by the abstract ground graph

Relational *d*-separation is sound and complete

Proof sketch

(1) *d*-separation for DAGs is sound [Verma & Pearl 1988] and complete [Geiger & Pearl 1988]

(2) Abstract ground graphs are directed and acyclic

- (3) Abstract ground graphs are sound and complete
- (4) Abstract ground graph completeness \Rightarrow Relational *d*-separation soundness
- (5) Abstract ground graph soundness \Rightarrow Relational *d*-separation completeness Valid up to a specified hop threshold *h*

Naïvely applying *d*-separation is frequently incorrect

Synthetic generation:

Schemas: |Entity classes | ∈ [1, 4]
Models: |Dependencies | ∈ [1, 10]
3.6 million pairs of relational variables

UNREPRESENTABLE (56%)

REPRESENTABLE (44%)

Unrepresentable: Either the treatment or outcome relational path includes an item class more than once.

E.g, [Employee, Develops, Product, Develops, Employee]

Naïvely applying *d*-separation is frequently incorrect



Most representable queries are marginally independent because the total dependencies varies from 1 to 15. Naïvely applying *d*-separation is frequently incorrect



Future work

- Include deterministic/functional dependencies (D-separation)
- Reason about models of entity and relationship existence
- Develop the implications of relational *d*-separation and abstract ground graphs (next—the RCD algorithm!)
Questions?

Topics

✓ Background on relational data and models

✓ Relational *d*-separation

The RCD algorithm



Markov equivalence class

Relational analog



Abstract ground graphs enable new constraints



Abstract ground graphs enable new constraints



Relational bivariate orientation (RBO)

• RBO leverages relational dependencies that cross relationships with a **MANY cardinality**.



- Assumes only model acyclicity (no assumptions about functional form or conditional densities).
 - Other bivariate dependency orientation methods can be used where RBO cannot [Shimizu et al. 2006; Hoyer et al. 2009; Zhang & Hyvärinen 2009; Peters et al. 2010].
- RBO can be described as detecting relational autocorrelation [Jensen & Neville 2002] and testing if a distinct variable is a member of the separating set that eliminates the autocorrelation.

Relational bivariate orientation (RBO)

Abstract ground graph from *I***^X perspective**



Does [I_X ... I_Y].Y help remove autocorrelation? $[I_X ... I_Y].Y \in sepset([I_X].X, [I_X ... I_Y ... I_X].X)?$

Orient as **Orient** as common effect common cause $[I_X].X \qquad [I_X...I_Y...I_X].X \quad [I_X].X \qquad [I_X...I_Y...I_X].X$ $[I_X \dots I_Y].Y$ $[I_X \dots I_Y].Y$

Extending PC orientation rules relationally



Known Non-Colliders (KNC)



Extending PC orientation rules relationally





Orientation propagation

 A single relational dependency supports many edges within and across the set of abstract ground graphs for a relational model.



 When a rule is activated for a specific abstract ground graph, the orientation of the underlying relational dependency must be propagated within and across all abstract ground graphs.

Orientation rule soundness and completeness

Soundness definition: An orientation rule is *sound* if any orientation not indicated by the rule introduces either

- (1) An unshielded collider in some abstract ground graph
- (2) A directed cycle in some abstract ground graph
- (3) A model-level cycle [Adapted from Meek 1995]

Completeness definition: A set of orientation rules is *complete* if any orientation of an unoriented edge is consistent with a member of the Markov equivalence class. [Meek 1995]

Proof: Shown for individually for soundness and collectively for completeness (CD, KNC, CA, MR3, RBO, and propagation)

The relational causal discovery algorithm

Initialize set of potential dependencies

Phase I: Identify skeleton via separating sets

Phase II: Build abstract ground graphs and orient dependencies

ALGORITHM 1: RCD(schema, depth, hopThreshold, P) 1 $PDs \leftarrow getPotentialDeps(schema, hopThreshold)$ 2 $N \leftarrow initializeNeighbors(schema, hopThreshold)$ **3** $S \leftarrow \{\}$ // Phase I 4 for $d \leftarrow 0$ to depth do for $X \to Y \in PDs$ do $\mathbf{5}$ foreach $condSet \in powerset(N[Y] \setminus \{X\})$ 6 do if |condSet| = d then 7 if $X \perp \!\!\!\perp Y \mid condSet$ in P then 8 $PDs \leftarrow PDs \setminus \{X \to Y, Y \to X\}$ 9 $S[X,Y] \leftarrow condSet$ $\mathbf{10}$ break 11 // Phase II **12** $AGGs \leftarrow \texttt{buildAbstractGroundGraph}(PDs)$ **13** $AGGs, S \leftarrow ColliderDetection(AGGs, S)$ 14 $AGGs, S \leftarrow \texttt{BivariateOrientation}(AGGs, S)$ 15 while changed do $AGGs \leftarrow \texttt{KnownNonColliders}(AGGs, S)$ 16 $AGGs \leftarrow CycleAvoidance(AGGs, S)$ 17 $AGGs \leftarrow \texttt{MeekRule3}(AGGs, S)$ 18 **19** return getCanonicalDependencies(AGGs)

RCD correctness

RCD correctly learns a maximally oriented model

Assumptions

- (1) Sufficient hop threshold *h*
- (2) Sufficient depth
- (3) Causal sufficiency
- (4) Faithfulness
- (5) Perfect conditional independence tests

Proof

Follows similarly to PC Phase I correctness and edge orientation rule completeness

Empirical evaluation

Synthetic model structure generation

- | Entity classes | \in [1, 4]
- |Relationship classes | = |Entity classes | 1
- |Attributes| ~ $Pois(\lambda=1) + 1$
- | Dependencies | \in [1, 15]

Algorithms

- RCD
- Relational PC (RPC) [Maier et al. 2010]
- Propositionalized PC (PPC)—best and worst perspectives
- (All using a relational *d*-separation oracle)

Evaluation measures



- For skeleton and oriented model

Identifying (causal) skeletons



Orienting dependencies



The unique contribution of RBO



Learning a causal model of the movie industry



Learning a causal model of the movie industry



Future work

- Develop more accurate tests of conditional independence for relational data
- Learn causal models of relationship existence
- Relax causal sufficiency by incorporating the relational blocking operator [Rattigan, Maier & Jensen 2011]
- Learn causal relational models with temporal dynamics

Summary

- Bayesian networks, *d*-separation, and the PC algorithm have provided a solid foundation for research on causal structure learning
- We now have an analogous basis for causal structure learning from relational data New representation (abstract ground graphs), capabilities for reasoning about independence (relational d-separation), and a sound and complete algorithm (RCD)

Thank you! Questions? maier@cs.umass.edu http://kdl.cs.umass.edu/rcd