Constraints on marginalized DAGs and their uses.

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Algebraic Statistics Workshop, NIMS
17th July 2014

Outline

Correlation does not imply causation

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How a short nap can raise the risk of diabetes: Study finds people who have a siesta are more likely to have high blood pressure and high cholesterol

- **Napping for more than 30 minutes at a time can raise the risk of diabetes, according to a new study**
- **It can also increase likelihood of high blood pressure and high cholesterol**

By PAT HAGAN

PUBLISHED: 01:04, 21 September 2013 | **UPDATED:** 10:34, 21 September 2013

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They were much favoured by Margaret Thatcher, Albert Einstein and Winston Churchill.

But while afternoon naps may revitalise tired brains, they can also increase the risk of diabetes, according to new research.

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Original Article

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[a] Ministry of Education Key Laboratory of Environment and Health, School of Public Health, Tongji Medical College, Huazhong University of Science and Technology, China

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[c] Department of Social Medicine, School of Public Health, Tongji Medical College, Huazhong University of Science and Technology, China

[d] Dongfeng General Hospital, Dongfeng Motor Corporation and Hubei University of Medicine, China

Abstract

Objectives

Afternoon napping is a common habit in China. We used data obtained from the Dongfeng–Tongji cohort to examine if duration of habitual afternoon napping was associated with risks for impaired fasting plasma glucose (IFG) and diabetes mellitus (DM) in a Chinese elderly population.

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> "Dr Matthew Hobbs, head of research for Diabetes UK, said there was no proof that napping **actually caused** diabetes."

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Distinguishing Between Causal Models

But can we still tell what causes what from observational data?

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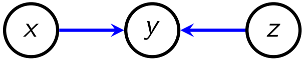

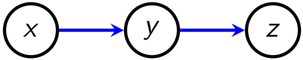

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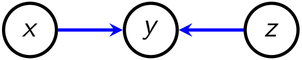

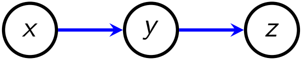

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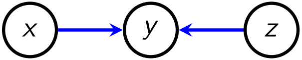

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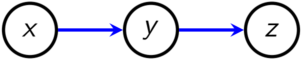

$X \perp\!\!\!\perp Z \mid Y$

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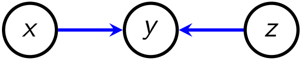

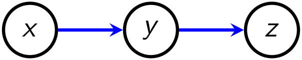

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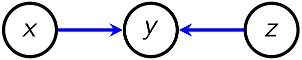

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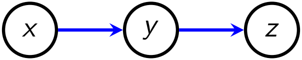

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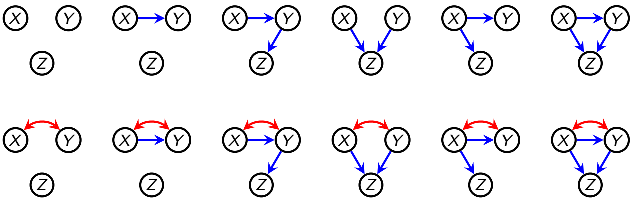
In order to do this well, we need to understand in what ways causal models will be **observationally** different.

Structure Learning

Given a distribution P (or rather data from P) and a set of possible causal models...



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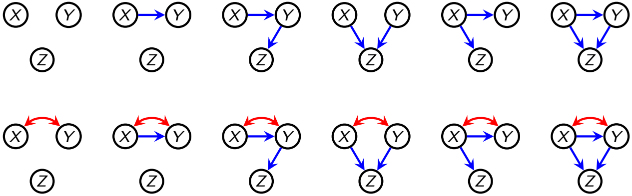

...return list of models which are compatible with data.

We can do this by testing whether constraints implied by the model(s) are satisfied by P. e.g. PC, FCI algorithms.

To do this we need to know what the constraints are (the focus of this talk).

Outline

1. Introduction
2. Conditional Independence and Algebraic Models
3. DAGs
4. Margins of DAG Models
5. Ordinary Markov Model
6. Verma Constraints
7. Results
8. Inequalities
9. Summary

Outline

Models for Contingency Tables

Take finite discrete random variables $X_V = (X_1, \ldots, X_n)$.

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Take finite discrete random variables $X_V = (X_1, \ldots, X_n)$.

For $x_V = (x_1, \ldots, x_n)$, joint distribution is parameterized by

$$p(x_V) = p(x_1, \ldots, x_n) = P(X_1 = x_1, \ldots, X_n = x_n).$$

We can consider a statistical model defined by polynomial constraints in the indeterminates $p(x_1, \ldots, x_n)$. We always assume

$$\sum_{x_V} p(x_V) = 1, \qquad\qquad p(x_V) > 0 \qquad \forall x_V.$$

Margins

For $M \subseteq V$, the **marginal distribution** over X_M is

$$p(x_M) = \sum_{x_{V \setminus M}} p(x_V) = \sum_{x_{V \setminus M}} p(x_M, x_{V \setminus M}).$$

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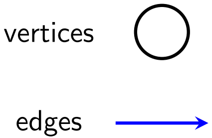
A **conditional independence** statement $X_A \perp\!\!\!\perp X_B \,|\, X_C$ assumes that $p(x_A \,|\, x_B, x_C) = p(x_A \,|\, x_C)$, or equivalently

$$p(x_A, x_B, x_C) \cdot p(x_C) - p(x_A, x_C) \cdot p(x_B, x_C) = 0$$

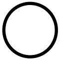
for all x_A, x_B, x_C.

Outline

Directed Acyclic Graphs

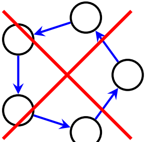


Directed Acyclic Graphs

vertices 

edges 

no directed cycles



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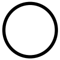
vertices 

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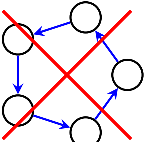

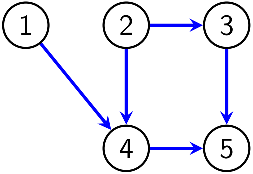

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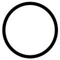
vertices 

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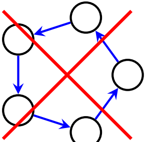
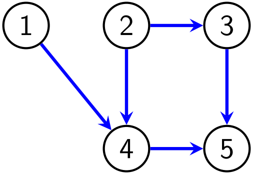




directed acyclic graph (DAG), $\mathcal{G}$

If $w \to v$ then w is a **parent** of v: $\mathrm{pa}_{\mathcal{G}}(4) = \{1, 2\}$.

If $w \to \cdots \to v$ then w is a **ancestor** of v: $\mathrm{an}_{\mathcal{G}}(5) = \{1, 2, 3, 4, 5\}$.

An **ancestral set** contains all its own ancestors.

DAG Models

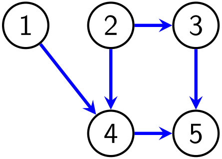
vertex		random variable
	$\iff$	X_a

DAG Models

vertex $\Longleftrightarrow$ random variable

X_a

graph $\mathcal{G}$ $\Longleftrightarrow$ model $\mathcal{M}$



$$\mathcal{M}(\mathcal{G}) = \{P \text{ satisfying } (*)\}$$

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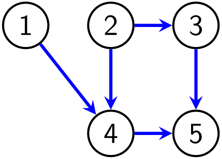

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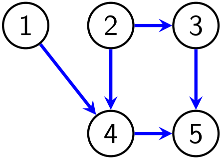
So in example above:

$$p(x_V) = p(x_1) \cdot p(x_2) \cdot p(x_3 \mid x_2) \cdot p(x_4 \mid x_1, x_2) \cdot p(x_5 \mid x_3, x_4)$$

Algebraic Models

Can also define model as a list of conditional independences:



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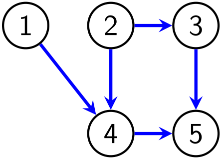

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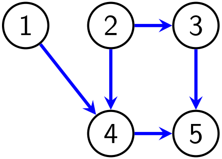

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So by identifying this with $(*)$, see the model is the same as setting

$$p(x_i \mid x_1, x_2, \ldots, x_{i-1}) = p(x_i \mid x_{\text{pa}(i)}), \qquad \text{for each } i.$$

Algebraic Models

Thus $\mathcal{M}(\mathcal{G})$ is precisely distributions such that:

$$X_i \perp\!\!\!\perp X_{[i-1]\setminus \mathrm{pa}(i)} \,|\, X_{\mathrm{pa}(i)}, \qquad\qquad i \in V.$$

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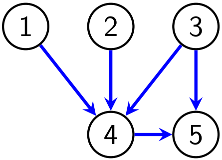

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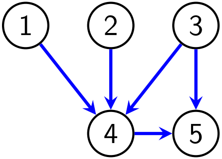

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So for discrete variables this is an algebraic model.

Structural Equation Model View

There is a second way to think about DAG models.

A distribution $P \in \mathcal{M}(\mathcal{G})$ iff[a] there exist functions f_i and independent variables E_i such that recursively setting

$$X_i = f_i(X_{\text{pa}(i)}, E_i)$$

gives X_V the distribution P.

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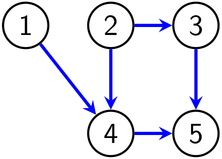

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X_4 &= f_4(X_1, X_2, E_4) \\
X_5 &= f_5(X_3, X_4, E_5).
\end{aligned}$$

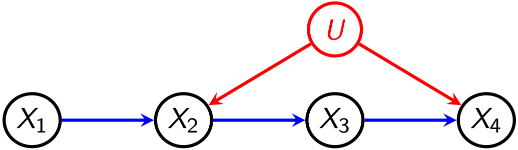
Reasons to Like DAG Models

- Induced constraints are all conditional independences: (reasonably) intuitive and simple to interpret;
- causal interpretation;
- modular structure is useful computationally and statistically;
- curved exponential families, known dimension;
- **algebraic model** for discrete variables.

Outline

Marginalization

Sometimes we cannot observe all the variables. Consider:



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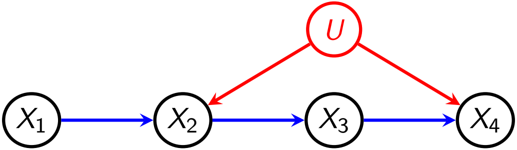

with U unobserved. This is a model defined (implicitly) by an integral:

$$p(x_1, x_2, x_3, x_4) = \int p(u)\, p(x_1)\, p(x_2 \mid x_1, u)\, p(x_3 \mid x_2)\, p(x_4 \mid x_3, u)\, du$$

We do **not** assume U is discrete, since we cannot observe it.

Marginalization

What we consider is **not** a latent variable model in the usual sense. **No state-space is assumed** for hidden variables (though uniform on $(0,1)$ is sufficient).

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But:

- cannot directly test membership of the model;
- model is complicated (as we shall see);
- not even clear it is a (semi-)algebraic model.

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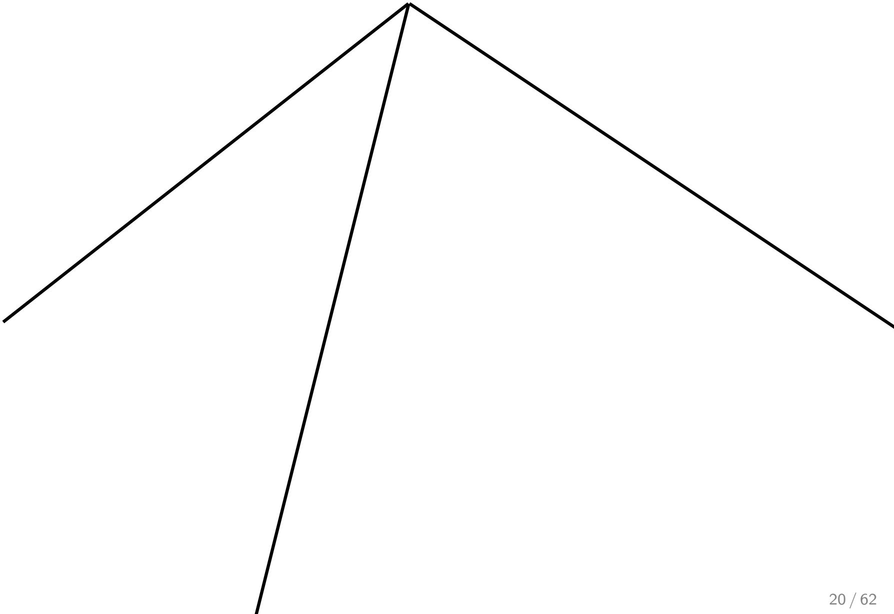
We aim to study the set of distributions constructed in this way.

Strategy: find some constraints satisfied by these models, define a new larger model using these constraints, and study that.

Getting the Picture



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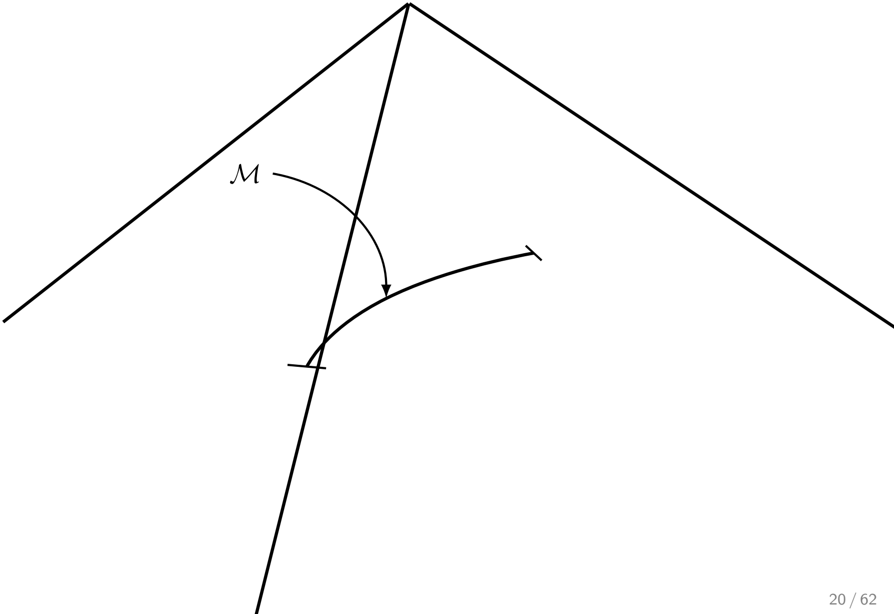

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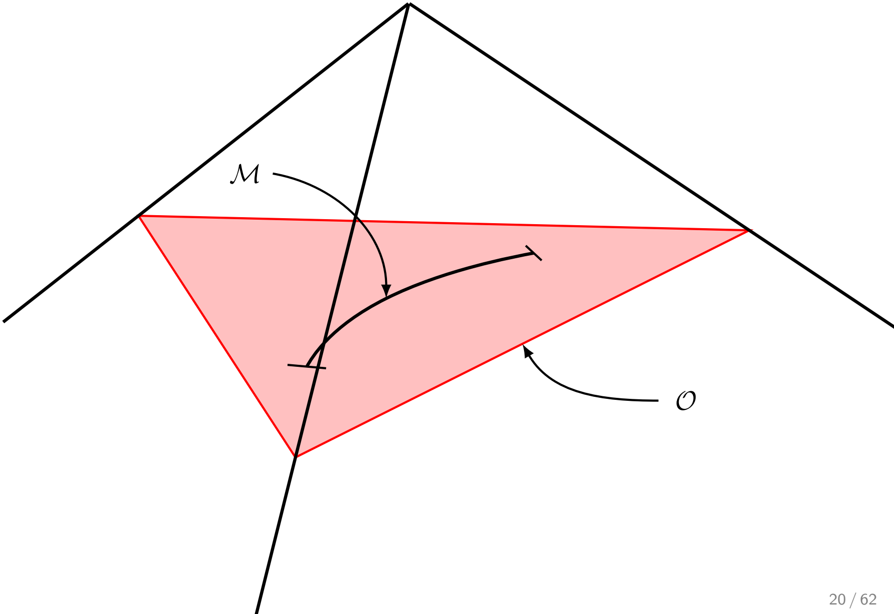

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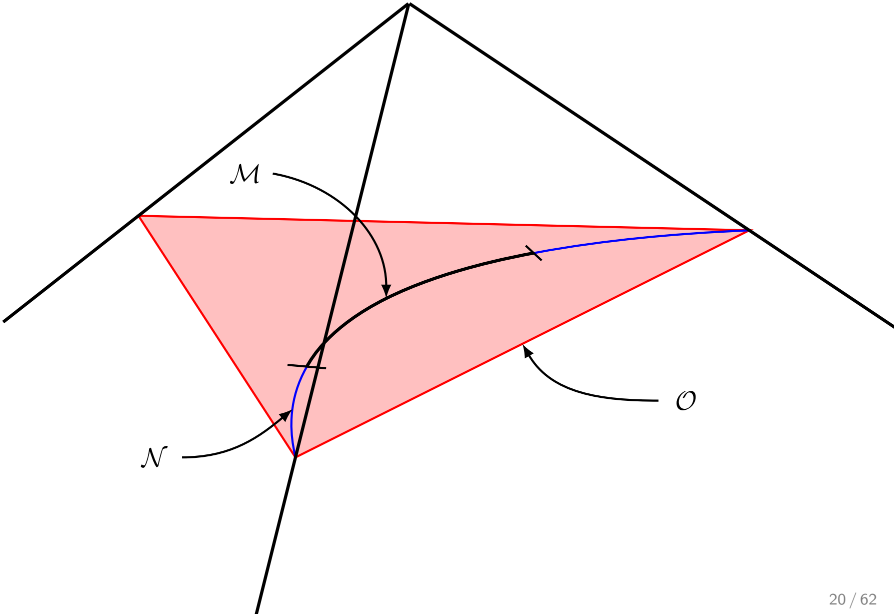

Latent Variable Models

Traditional latent variable models would assume that the hidden variables are discrete with some fixed number of states.

Advantages: semi-algebraic model after eliminating variables is semi-algebraic, and can fit with (e.g.) EM algorithm.

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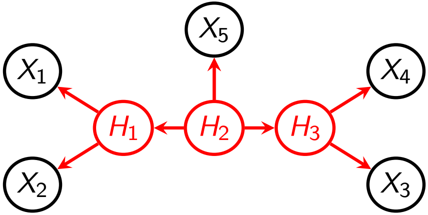
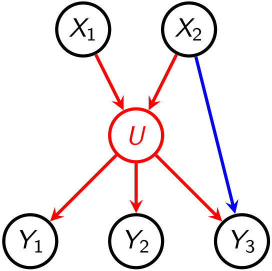


But: latent variables lead to singularities and nasty statistical properties (see e.g. Drton, Sturmfels and Sullivant, 2009)

Simplifications

Simplification 1. WLOG latents vertices have no parents.



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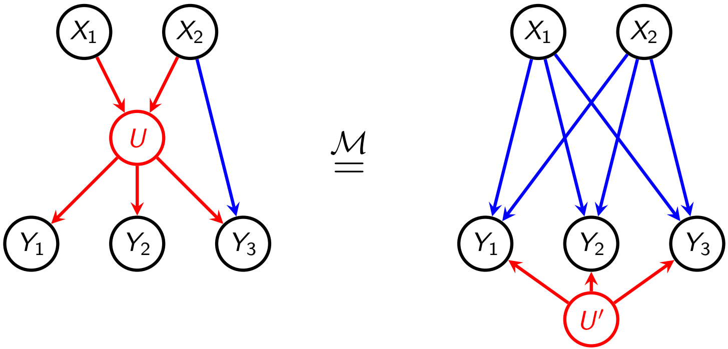

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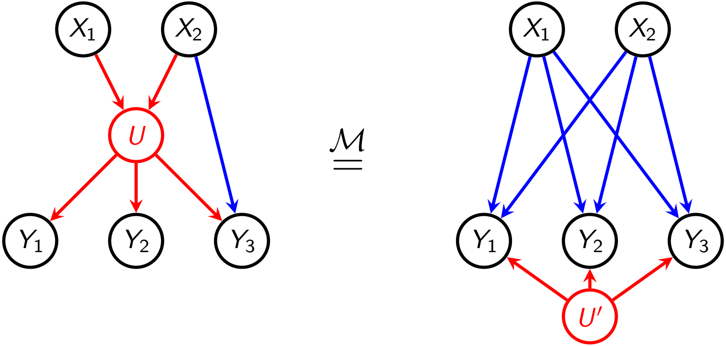
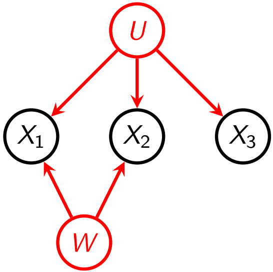


(Of course, this is not true if we assume a specific state-space: e.g. phylogenetic model)

Simplifications

Simplification 2. If U, W are latent with $\mathrm{ch}_{\mathcal{G}}(W) \subseteq \mathrm{ch}_{\mathcal{G}}(U)$, then we don't need W.



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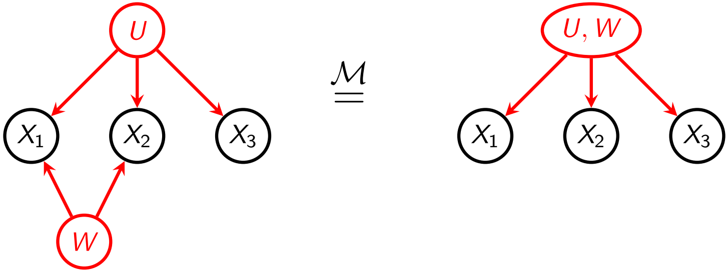
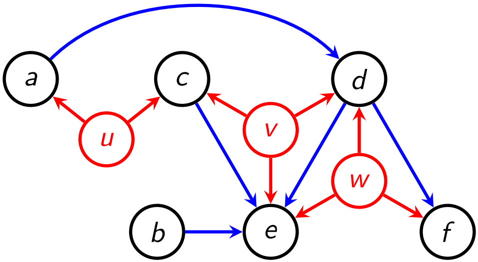


mDAGs

So we only need to consider models like this:



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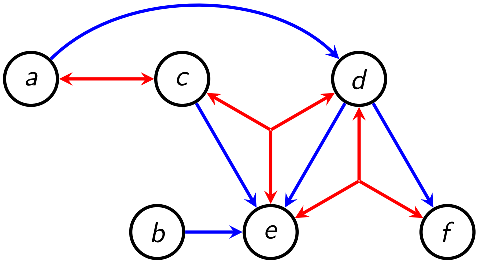

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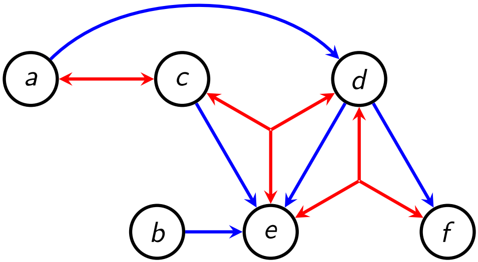

...which we represent with a hyper-graph called an **mDAG**.

The red edges $\leftrightarrow$ are called **bidirected**.

We want the set of distributions that can be obtained by the latent variable; this is the **complete model** $\mathcal{M}(\mathcal{G})$ for mDAG $\mathcal{G}$.

Geared Graphs

Call an mDAG **geared** if its bidirected edges satisfy the running intersection property.

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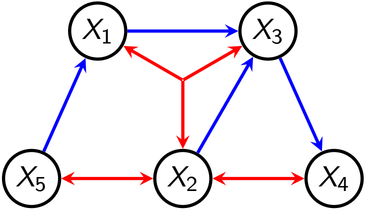
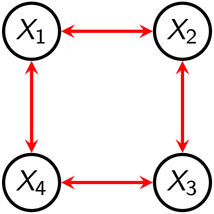
geared

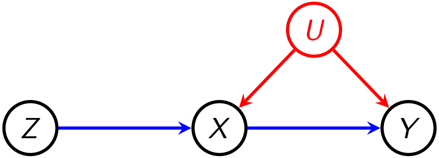


not geared



Functional Dependences

Consider the situation below.



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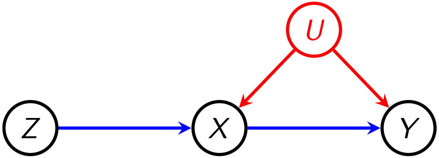

Recall the structural equation view: for some 'error' variables E_x, E_y:

$$X = f_X(Z, U, E_x) \qquad Y = f_Y(X, U, E_y).$$

Without loss of generality, can assume $U' = (U, E_x, E_y)$, so all additional randomness is contained in U'.

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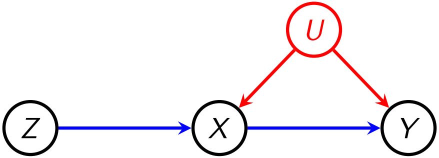

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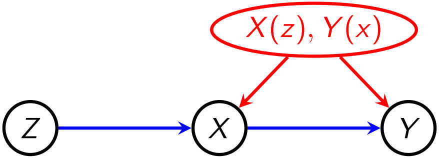

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Set $U = (X(z), Y(x))$, drawn from **finite** set of functions.

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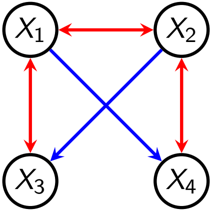

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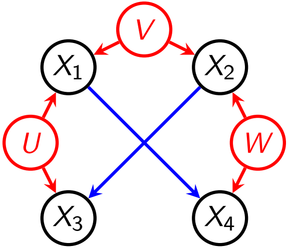

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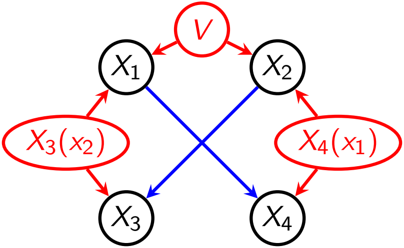

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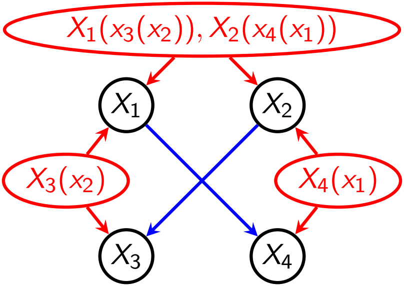

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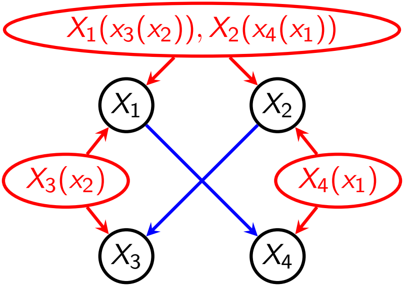

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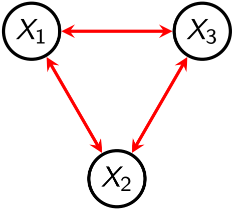
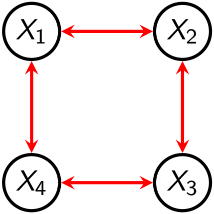
This representation turns out to be important in proving completeness of constraints.

Non-Geared Graphs

With a graph which is not geared, we cannot do this.





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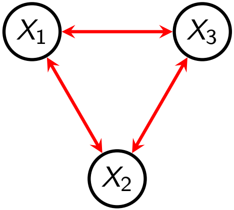
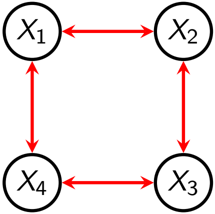


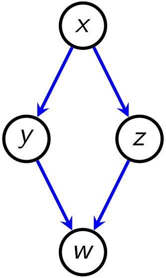


Open Problem: These models may or may not be semi-algebraic.

Outline

Ancestral Sets

Recall an **ancestral set** contains its own ancestors, e.g. $\{x, y, z\}$.



Marginalize w:

$$p(x, y, z) = \sum_{\mathbf{w}} p(x)\, p(y \mid x)\, p(z \mid x)\, p(\mathbf{w} \mid y, z)$$

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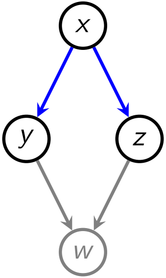

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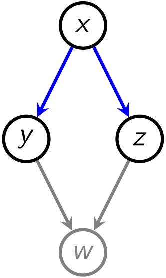

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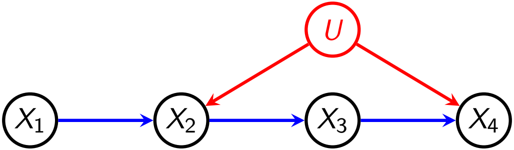
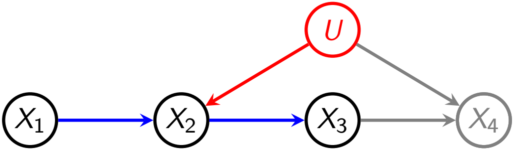
Models 'closed' under marginalization of vertices with no children.

Ancestral Sets



$$p(x_1, x_2, x_3, x_4)$$
$$= \int p(u)\, p(x_1)\, p(x_2 \mid x_1, u)\, p(x_3 \mid x_2)\, p(x_4 \mid x_3, u)\, du$$

Ancestral Sets



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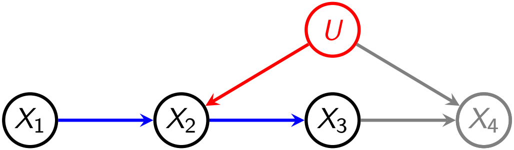

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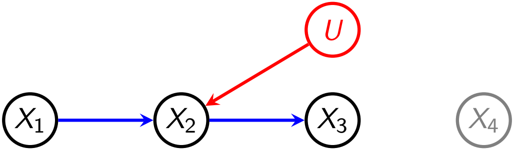

$$
\begin{aligned}
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&= \int p(u)\, p(x_1)\, p(x_2 \mid x_1, u)\, p(x_3 \mid x_2) \sum_{\mathbf{x_4}} p(\mathbf{x_4} \mid x_3, u)\, du \\
&= \int p(\mathbf{u})\, p(x_1)\, p(x_2 \mid x_1, \mathbf{u})\, p(x_3 \mid x_2)\, d\mathbf{u}
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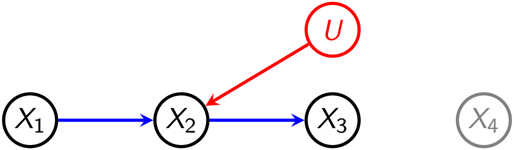

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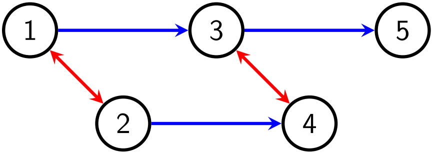
$$

gives $X_1 \perp\!\!\!\perp X_3 \mid X_2$.

Districts

Define a **district** in an mDAG to be maximal sets connected by latent variables:



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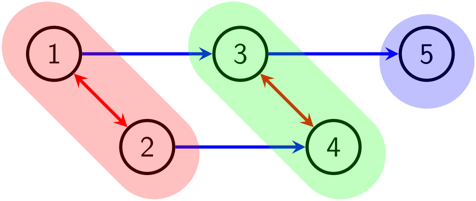

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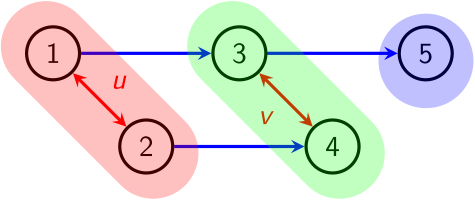

$$\int p(u)\, p(x_1 \mid u)\, p(x_2 \mid u) \quad p(v)\, p(x_3 \mid x_1, v)\, p(x_4 \mid x_2, v) \quad p(x_5 \mid x_3)\; du\, dv$$

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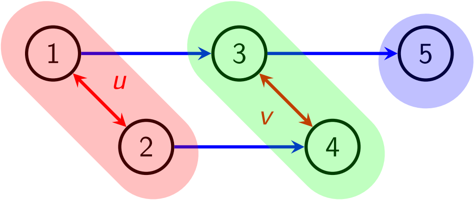

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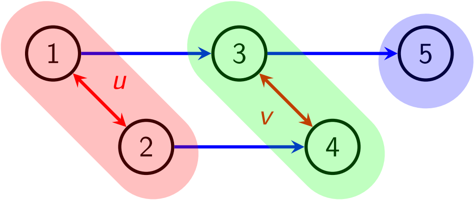

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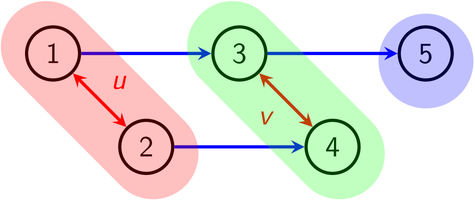

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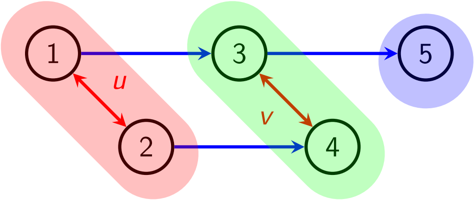

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$$= \prod_i q_{D_i}(x_{D_i} \mid x_{\mathrm{pa}(D_i)})$$

Axiomatic Approach

Define $\mathcal{O}(\mathcal{G})$ as set of P satisfying:

1. **Ancestrality:** $P \in \mathcal{O}(\mathcal{G})$ only if

$$\sum_{x_w} p(x_V) \in \mathcal{O}(\mathcal{G}_{-w})$$

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2. **Factorization into districts:** $P \in \mathcal{O}(\mathcal{G})$ only if

$$p(x_V) = \prod_D q_D(x_D \,|\, x_{\mathrm{pa}(D)})$$

   for districts D and some functions q_D.

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$$\sum_{x_w} p(x_V) \in \mathcal{O}(\mathcal{G}_{-w})$$

   for each childless w.

2. **Factorization into districts:** $P \in \mathcal{O}(\mathcal{G})$ only if

$$p(x_V) = \prod_D q_D(x_D \,|\, x_{\mathrm{pa}(D)})$$

   for districts D and some functions q_D.

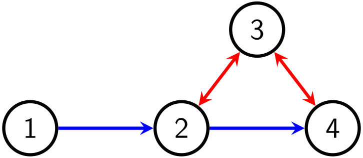
Call this the **ordinary Markov model** (OMM).

Properties of the OMM

First described by Richardson (2003, 2009); factorization and parametrizations in Evans and Richardson (2013, 2014).

- Strict superset of latent variable model;
- equivalent to taking all the conditional independences from the original model which only involve 'visible' variables;
- therefore algebraic (quadratic constraints in the probabilities);
- has parametrization, so irreducible variety;
- curved exponential families.

Example



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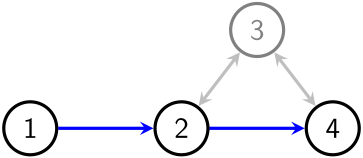

So $X_1 \perp\!\!\!\perp X_4 \mid X_2$

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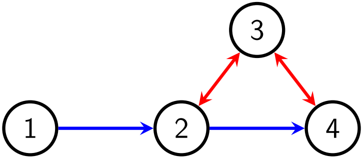

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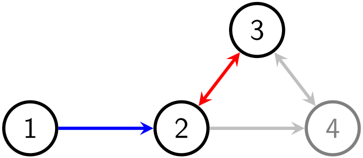

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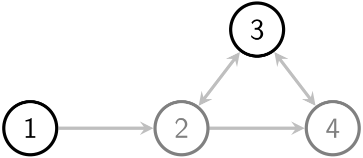
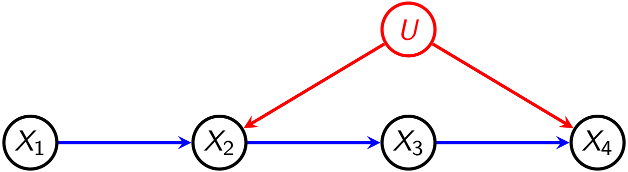


So $X_1 \perp\!\!\!\perp X_4 \mid X_2$ and $X_1 \perp\!\!\!\perp X_3$.

Outline

A Deficiency



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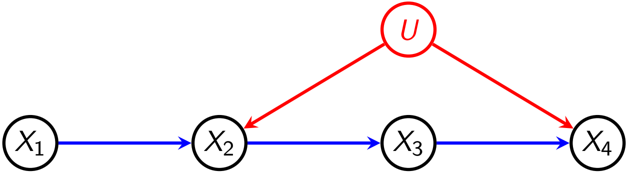

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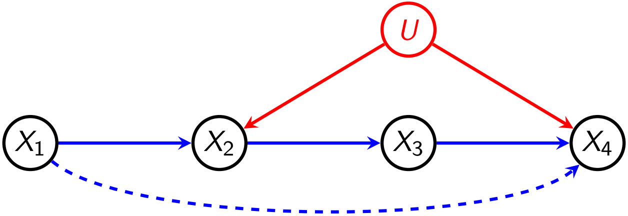
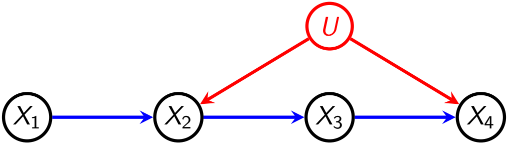


If U is latent, OMM gives only $X_3 \perp\!\!\!\perp X_1 \mid X_2$.

But if we add an arrow $X_1 \to X_4$, we still have $X_3 \perp\!\!\!\perp X_1 \mid X_2$.
So can we detect that $X_1 \not\to X_4$?

The Verma Constraint



$$p(x_1, x_2, x_3, x_4) = \int p(\mathbf{u})\, p(x_1)\, p(x_2 \mid x_1, \mathbf{u})\, p(x_3 \mid x_2)\, p(x_4 \mid x_3, \mathbf{u})\, d\mathbf{u}$$

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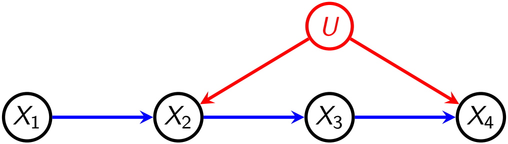

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(This is our district factorization.)

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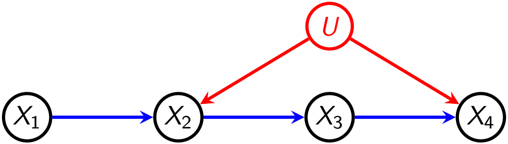

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&= p(x_1)\, p(x_3 \mid x_2)\, q(x_2, x_4 \mid x_1, x_3).
\end{aligned}
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(This is our district factorization.) But note that

$$
\begin{aligned}
\sum_{x_2} q(x_2, x_4 \mid x_1, x_3) &= \sum_{\mathbf{x_2}} \int p(u)\, p(\mathbf{x_2} \mid x_1, u)\, p(x_4 \mid x_3, u)\, du \\
&= p(x_4 \mid x_3)
\end{aligned}
$$

is independent of x_1, precisely because $X_1 \not\to X_4$.

Verma Constraints are Polynomials

This is the **Verma constraint** (Pearl and Verma, 1990):

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Note degree increases with number of states of X_1 and X_2.
Generally:

$$|\mathfrak{X}_1| + |\mathfrak{X}_2| \qquad \text{(or } |\mathfrak{X}_1|(1 + |\mathfrak{X}_2|)\text{)}$$

Reflects difficulty of estimating $p(x_1)$ and $p(x_3 \mid x_1, x_2)$ and dividing out by them(?)

Subgraphs

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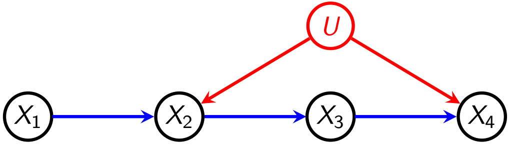

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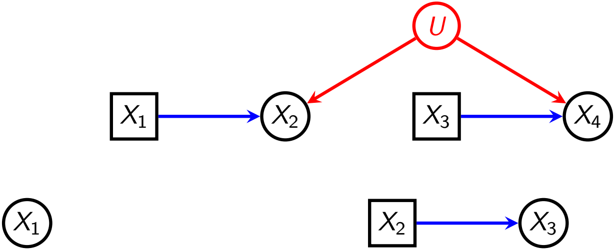

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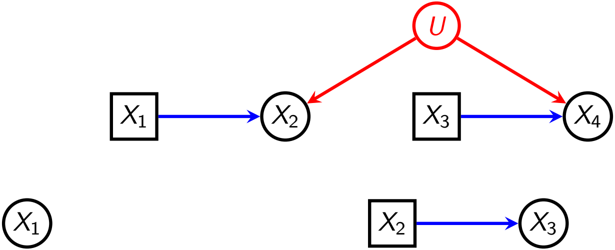
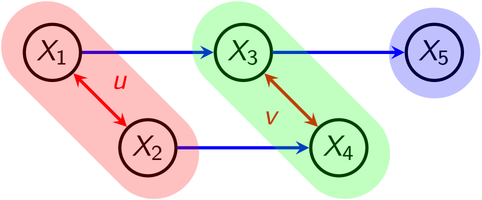


$$\frac{p(x_1, x_2, x_3, x_4)}{p(x_1) \cdot p(x_3 \mid x_2)} = \int p(u)\, p(x_2 \mid x_1, u)\, p(x_4 \mid x_3, u)\, du$$

So each factor of the distribution q_D corresponds to a 'piece' of the graph $\mathcal{G}[D]$.

Districts



$$\int p(x_1 \mid u)\, p(x_2 \mid u)\; p(x_3 \mid x_1, v)\, p(x_4 \mid x_2, v)\; p(x_5 \mid x_3)\; du\, dv$$

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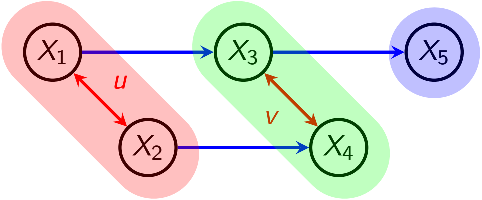

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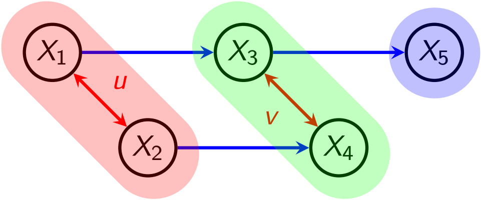

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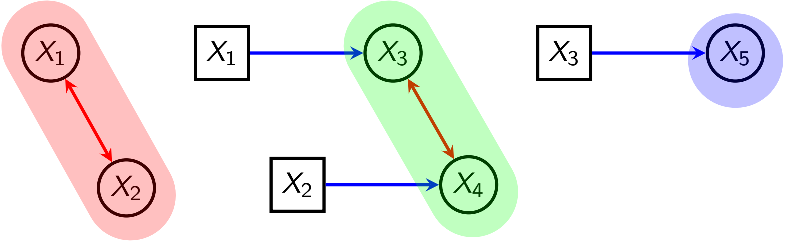
The form of each q is important.

Districts



$$\int p(u)\, p(x_1 \mid u)\, p(x_2 \mid u)\; p(v)\, p(x_3 \mid x_1, v)\, p(x_4 \mid x_2, v)\; p(x_5 \mid x_3)\, du\, dv$$

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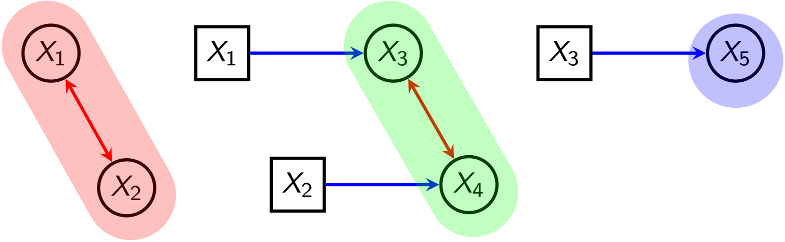

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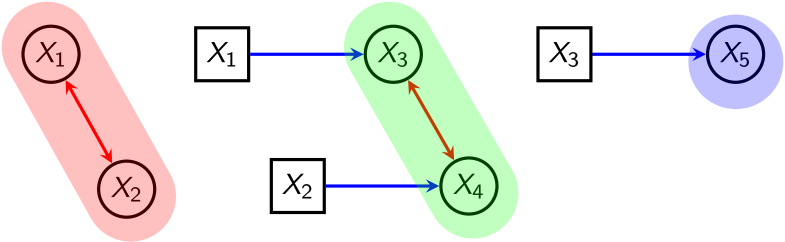

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$$= q(x_1, x_2) \cdot q(x_3, x_4 \mid x_1, x_2) \cdot q(x_5 \mid x_3).$$

$$= \prod_i q_{D_i}(x_{D_i} \mid x_{\mathrm{pa}(D_i)})$$

Each q_D piece should come from the model based on district subgraph and its parents ($\mathcal{G}[D]$).

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Define $\mathcal{N}(\mathcal{G})$ as a model satisfying:

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Call this the **nested Markov model** (NMM).

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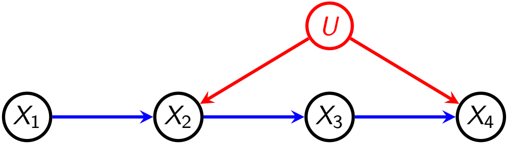

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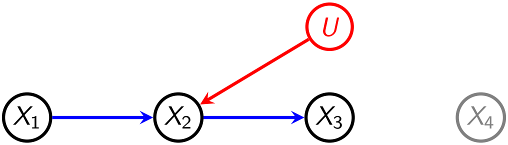

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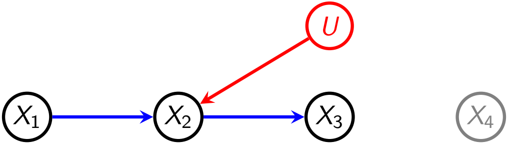

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and therefore $X_1 \perp\!\!\!\perp X_3 \,|\, X_2$.

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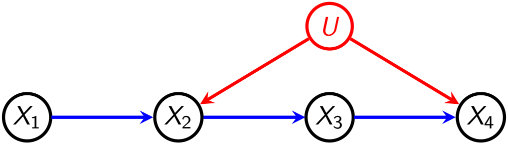

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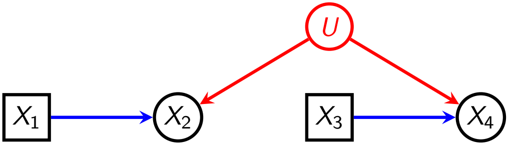

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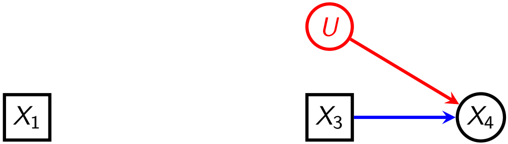

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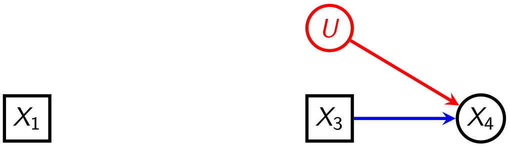

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We see that $X_1 \perp\!\!\!\perp X_3, X_4\,[q_{24}]$.

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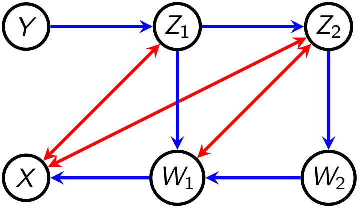
In the below example, X and Y are not adjacent: is there a constraint implied?



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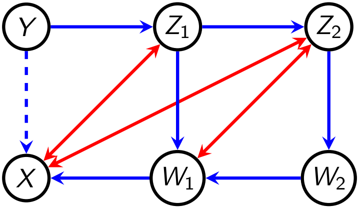

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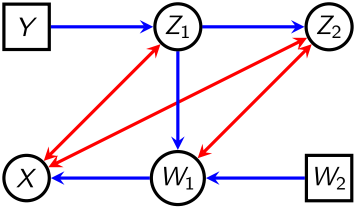

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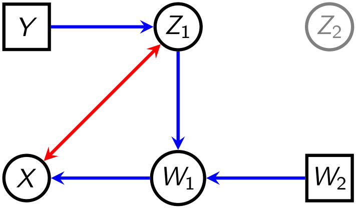

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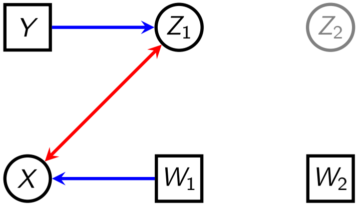

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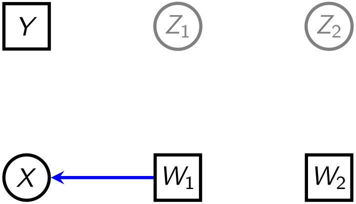

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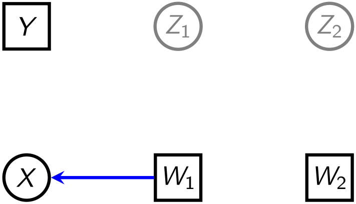

So $X \perp\!\!\!\perp Y \mid W_1$ in a twice re-weighted distribution P^{**}.

So can distinguish between these two structures...
...but this is a degree-12 polynomial!

Outline

Main Result

How do we know there isn't **another** 'axiom' we could use?

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Theorem (Evans)

For any discrete DAG model, the nested and complete Markov models are algebraically equivalent (i.e. same dimension):

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This has very nice statistical implications.

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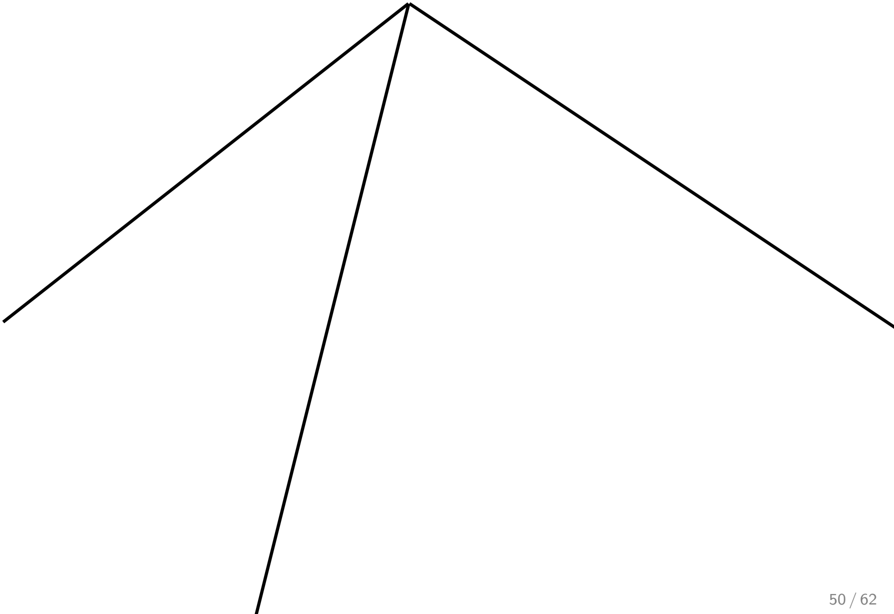

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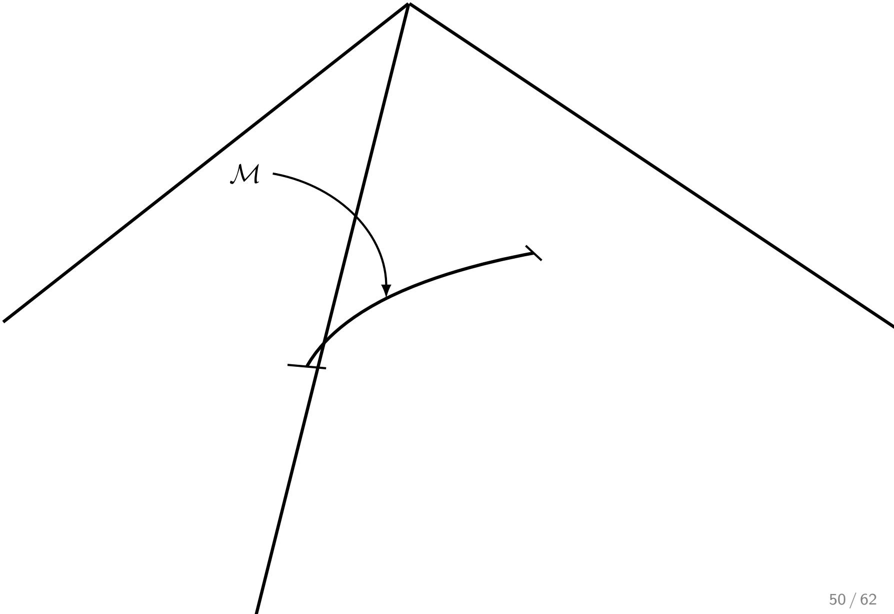

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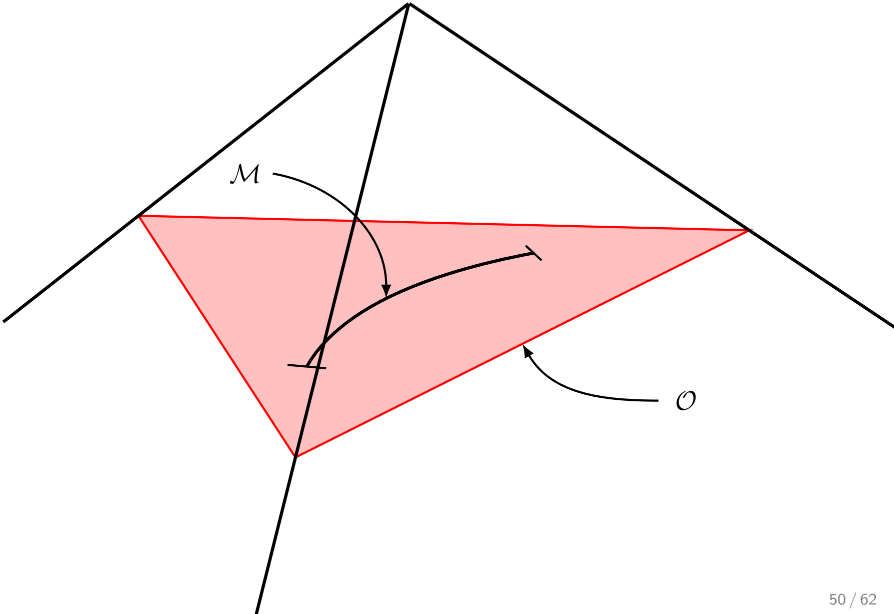

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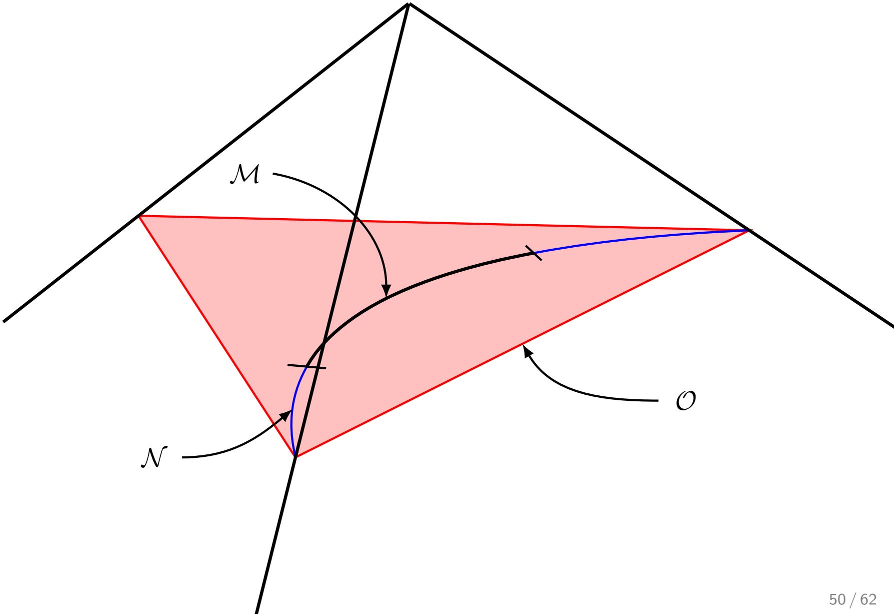
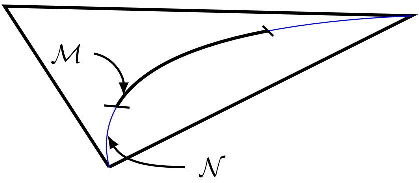


Proof idea for main result

- The nested model can be defined parametrically;



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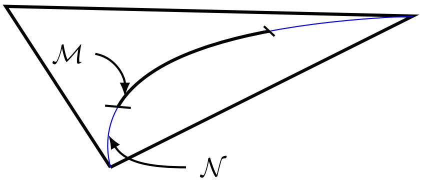

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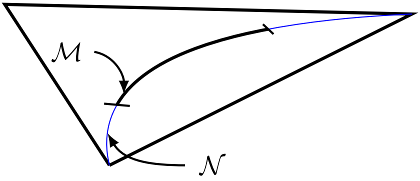

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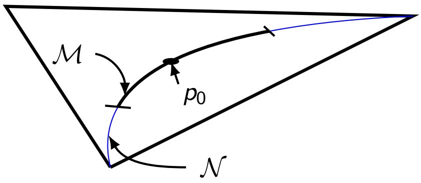

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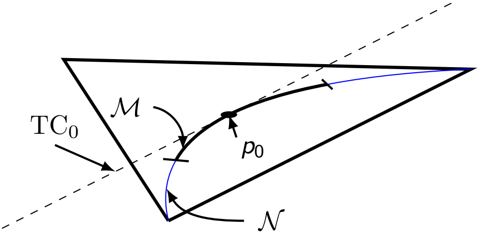
- hence if, in a neighbourhood of a single point, the nested and complete models are the same dimension, then they have the same Zariski closure;
- the uniform distribution (complete independence, all states equally likely) is contained in any mDAG model;
- we can perturb the relationship between latent and observed variables to 'move' $\mathcal{M}$ in any direction within the tangent space of $\mathcal{N}$.



Proof Outline

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$$D \subseteq A \cup B \cup C, \quad D \cap A \neq \emptyset, \quad D \cap B \neq \emptyset.$$

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If $X_A \perp\!\!\!\perp X_B \,|\, X_C$ under $\mathcal{M}$, then $\Lambda_D \perp TC_0(\mathcal{M})$ for D as above.

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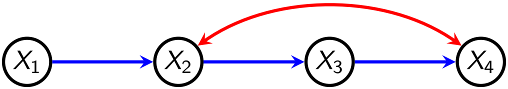
In fact, this is true even for a dormant independence.

Verma Example



We have $X_1 \perp\!\!\!\perp X_3 \mid X_2$ and (after a re-weighting) $X_1 \perp\!\!\!\perp X_4 \mid X_3$.

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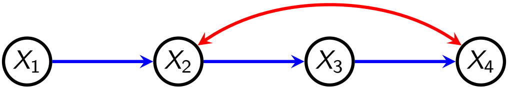

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Hence $\Lambda_{13} + \Lambda_{123} + \Lambda_{14} + \Lambda_{134} \perp TC_0(\mathcal{M})$.

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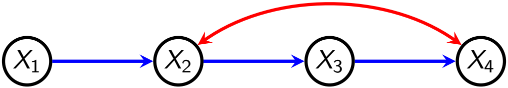

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So: need to show all the *other* spaces λ_A are inside the tangent cone.

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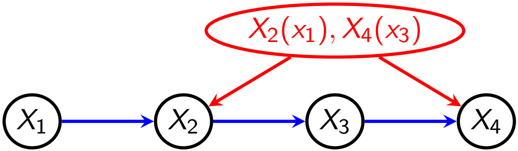

Perturbing	controls
X_1	Λ_1
$X_3 \mid X_2$	$\Lambda_3 + \Lambda_{23}$
$X_2(x_1)$	$\Lambda_2 + \Lambda_{12}$
$X_4(x_3)$	$\Lambda_4 + \Lambda_{34}$
$X_2(x_1), X_4(x_3)$ *jointly*	$\Lambda_{24} + \Lambda_{124} + \Lambda_{234} + \Lambda_{1234}$

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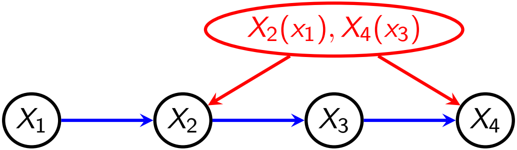

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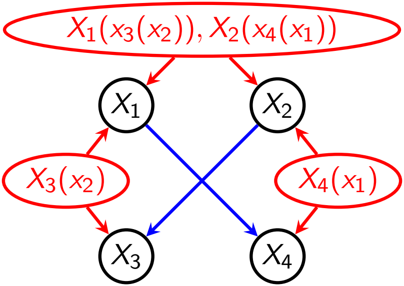
$\Lambda_{13}, \Lambda_{123}, \Lambda_{14}, \Lambda_{134}$ are constrained, so that's all of them!

Geared Graphs

Back to our harder example:



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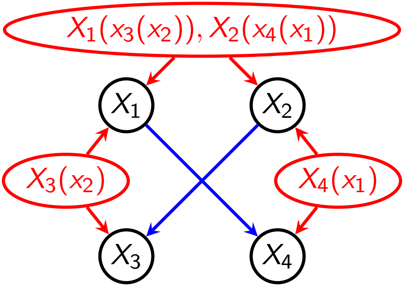

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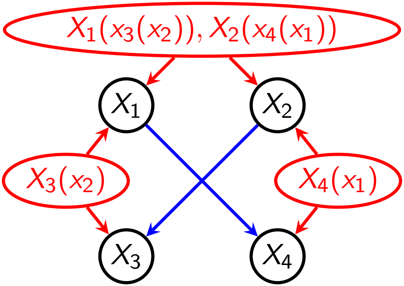

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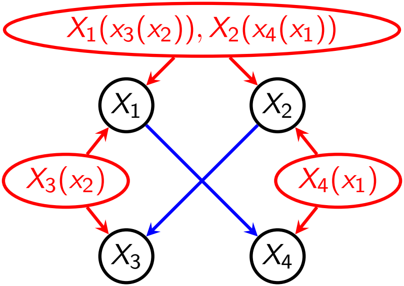

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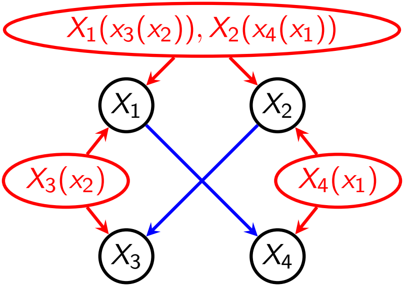

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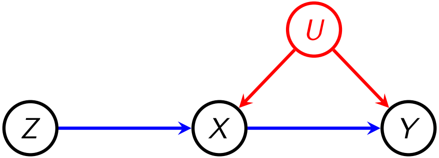
Outline

Inequality Results



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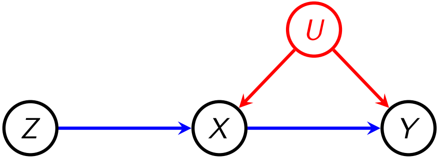

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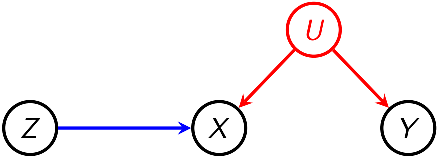

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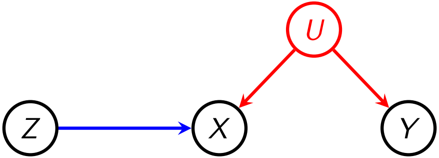

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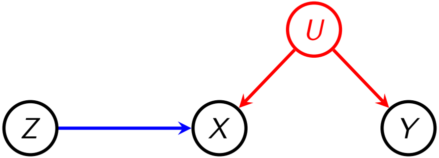

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This 'compatibility' requirement turns out to place an inequality restriction on p: $$\max_x \sum_y \max_z p(x, y \mid z) \leq 1.$$

Inequality Results

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Maybe the nested model is a good compromise!

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Summary

We have seen that:

- we can provide graphical derivations of constraints on DAG models; this leads to:
  - **(i)** the ordinary Markov model (conditional independences);
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- statistical and practical properties generally better than latent variable models;
- we can also give graphical derivations for some inequalities.

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We've dealt with marginalization, but what about conditioning?

Thank you!

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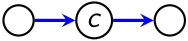

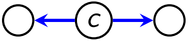

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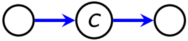
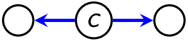
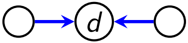
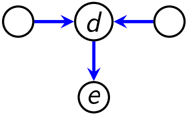




(ii) or any collider is not in C, nor has descendants in C:



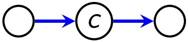


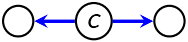
d-Separation

A **path** is a sequence of edges in the graph; vertices may not be repeated.

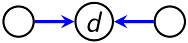
A path from a to b is **blocked** by $C \subseteq V \setminus \{a, b\}$ if either

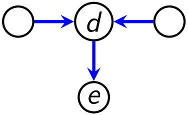
(i) any non-collider is in C:





(ii) or any collider is not in C, nor has descendants in C:





Two vertices a and b are **d-separated** given $C \subseteq V \setminus \{a, b\}$ if **all** paths are blocked.

Parameterizations

The nested and ordinary Markov models are also defined by

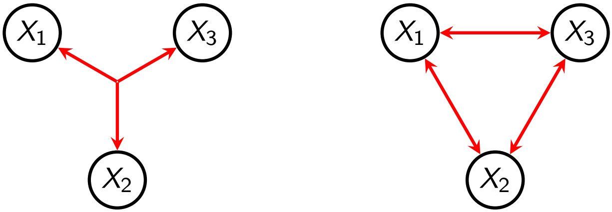
$$P(X_V = x_V) = \sum_{O \subseteq C \subseteq V} (-1)^{|C \setminus O|} \prod_{H \in [C]_{\mathcal{G}}} q_H(x_T).$$

for some pairs of sets (H, T), and partitioning function $[\cdot]_{\mathcal{G}}$. (See Evans and Richardson, 2014, for details)

Note the form is the same for the ordinary and nested models, but the partitioning function differs (as does the interpretation of the parameters q).

ADMGs are not sufficient

In general we need to distinguish between $\{1,2,3\}$ and $\{1,2\}$, $\{1,3\}$, $\{2,3\}$.



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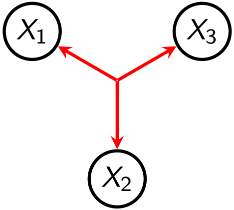

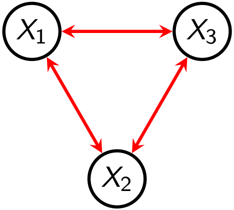

The model on the right is not saturated. Still true if we dichotomize.

ADMGs are not sufficient

Lemma

Let $\mathcal{F}$, $\mathcal{G}$, $\mathcal{H}$ be mutually independent σ-algebrae (so that $\mathcal{F} \perp\!\!\!\perp \mathcal{G} \vee \mathcal{H}$ and so on), and let X, Y and Z be random variables such that

(i) X is $\mathcal{F} \vee \mathcal{G}$-measureable;

(ii) Y is $\mathcal{G} \vee \mathcal{H}$-measureable;

(iii) Z is $\mathcal{F} \vee \mathcal{H}$-measureable.

Then $P(X = Y = Z) > 1 - \epsilon$ implies

$$\operatorname{Var} X < 3\epsilon.$$