Non-probabilistic Markov Categories for Causal Modeling in Machine Learning

Dhurim Cakiqi[1] Max A. Little[1,2]

[1]School of Computer Science,
University of Birmingham, UK

[2]Media Lab,
MIT,USA

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Outline

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The limitation of machine learning

- Machine learning (ML) is very useful in modeling large data sets
- Typically machine learning is non-probabilistic
- This is a "causally-blind" approach to modeling
- We need a method which takes into account the possibility of spurious correlations in the data

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Causal modeling

What is it?

- It is a probabilistic method in which to model the causal influence of events on another
- Typically, it is represented by a directed acyclic graph (DAG)
- $A \rightarrow B$ represents A having a causal influence on B
- Given an arbitrary DAG the probability distribution is given by

$$P\left(X_1, \ldots, X_n\right) = \prod_{n=1}^{N} P\left(X_n | \text{pa}\left(X_n\right)\right)$$

- In causal modeling the do-operator is used to simulate experimental interventions by changing the structure of the DAG
- The interventional distribution $P\left(Y | \text{do}\left(X\right)\right)$ is computed after replacing all incoming arrows into X with the constant $X = x$.

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Back-door adjustment formula

- Suppose we were interested in the direct causal effect of a drug on a patient's health, and there is a confounder in the age of the patient
- We can represent this in a DAG by,

$$H \leftarrow A \rightarrow D$$

$$D \rightarrow H$$

- In this case we make use of the *back-door adjustment* formula

$$P\left(H|\text{do}\left(D=d\right)\right)=\sum_{a\in\Omega_A}P\left(H|A=a,D=d\right)P\left(A=a\right).$$

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The need for semifields

- In order to normalize we need an algebra that has a multiplicative inverse and for our purposes additive inverses are not required
- Semifields are critical so that we can form a consistent set of rules in order to manipulate casual morphisms
- Semifields can be used to represent machine learning models, e.g. ML and deep learning (DL) algorithms.

Example

(Probability semifield). $([0,1], +, \times, 0, 1)$

Example

(Min-plus semifield). $(\mathbb{R}^{+}, \min, +, \infty, 0)$

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Semifields

Definition

A semifield $(S, \oplus, \otimes, i_\oplus, i_\otimes)$, is a set, S, endowed with two binary operations $\oplus, \otimes$ that satisfy the following conditions;

1. $\oplus$ is associative and commutative on all $a, b \in S$ and has identity $i_\oplus$ i.e. $\forall a \in S, i_\oplus \oplus a = a \oplus i_\oplus = a$
2. $\otimes$ is associative and has identity $i_\otimes$ i.e. $\forall a \in S, i_\otimes \otimes a = a \otimes i_\otimes = a$, and for all $a \in S \setminus \{i_\oplus\}$ there exists an inverse a^{-1} such that $a \otimes a^{-1} = a^{-1} \otimes a = i_\otimes$
3. $\otimes$ is both left and right distributive with respect to $\oplus$ and for every $s \in S$, $i_\oplus$ annihilates s, i.e. $a \otimes i_\oplus = i_\oplus \otimes a = i_\oplus$.

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Defining the category

Definition

A Markov category **C** is a symmetric monoidal category in which every object $X \in \mathbf{C}$ is equipped with a commutative comonoid structure given by a comultiplication $\mathrm{copy}_X : X \to X \times X$ and counit $\mathrm{del}_X : X \to I$, where $\times$ is the tensor product and I is the unit object. The comultiplication and counit are usually depicted in string diagrams, further they satisfy commutative comonoid equations, compatibility with the monoidal structure and the naturality of del.

Definition

A *semifield* Markov category **C** is a Markov category in which morphism composition and the monoidal product is defined by some underlying semifield $(S, \otimes, \oplus, i_\otimes, i_\oplus)$. A special case of this category is the *affine semifield* Markov category in which there is an associated terminal morphism for each object $X \in \mathbf{C}$.

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Defining the category

Extra structure

Objects, morphisms and morphism composition

Objects in semifield Markov categories are arbitrary index sets X, Y, and morphisms are of the form $\mathbf{f} : X \to D(Y)$, where $D(Y) = S^Y$ i.e. the set of all maps $m : Y \to S$, D is as a monad. Morphism composition in the category denoted $\cdot$, on two morphisms $\mathbf{f}_1 : X \to D(Y)$ and $\mathbf{f}_2 : Y \to D(Z)$, is given as

$$(\mathbf{f}_1 \cdot \mathbf{f}_2)(z|x) = \bigoplus_{y \in Y} \mathbf{f}_2(z|y) \otimes \mathbf{f}_1(y|x).$$

The affine requirement

For two morphisms $\mathbf{f} : Z \to D(Y)$ and $\mathbf{1}_Y : Y \to D(1)$, composition of the two yields

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Marginalization, normalization, extraction and disintegration

Marginalization and normalization

Assume $\mathbf{C}$ is an affine semifield Markov over an arbitrary semifield $\mathbf{S} = (S, \oplus, \otimes, i_{\oplus}, i_{\otimes})$;

- *Marginalization*: For a morphism $\mathbf{f} : Z \to D(Y)$ and a terminal morphism $\mathbf{1}_Y : Y \to D(1)$, we have $\mathbf{1}_Y \cdot \mathbf{f} = \mathbf{1}_Z$ so that

$$\bigoplus_{y \in Y} [\mathbf{1}_Y(|y) \otimes \mathbf{f}(y|z)] = \mathbf{1}_Z(|z).$$

- *Normalization*: For a morphism $\mathbf{f} : X \to D(Y)$ we define a normalized morphism with a bar i.e. $\bar{\mathbf{f}}(y|x)$ as follows,

$$\bar{\mathbf{f}}(y|x) = \mathbf{f}(y|x) \otimes \left(\bigoplus_{y \in Y} \mathbf{f}(y|x) \right)^{-1},$$

where $\mathbf{f}(y|)$ denotes a morphism with no input and $\mathbf{f}(|y)$ is a morphism with no output.

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Extraction and disintegration

Let $\times$ denote the monoidal product in which for two arbitrary morphisms $\mathbf{f} : X \to D(Y)$ and $\mathbf{g} : Y \to D(Z)$ we have $\mathbf{f} \times \mathbf{g} = (\mathbf{f} \times \mathbf{g})(x, y | u, v)$;

- *Extraction*: For a morphism $\mathbf{f} : X \to D(Y)$, extraction is defined as

$$\mathbf{f}(x, y | z) \mapsto \bar{\mathbf{f}}(y | x, z).$$

- *Disintegration*: For a morphism $\mathbf{f}_{12} : 1 \to D(X_1 \times X_2)$, disintegration is given as

$$\mathbf{f}_{12}(x_1, x_2 |) = \bar{\mathbf{f}}_{1|2}(x_1 | x_2) \otimes \mathbf{f}_2(x_2 |),$$

where we have morphisms $\bar{\mathbf{f}}_{1|2}(x_1 | x_2) : X_2 \to D(X_1)$ and $\mathbf{f}_2(x_2 |) : 1 \to D(X_2)$.

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Example of morphisms and compositions from machine learning

State normalization under the min-plus semifield

Example

Let $\mathbf{g}(y|\lambda) = -\ln(\lambda) + \lambda y$ for $y \in Y = \mathbb{R}^+$ and $\lambda > 0$, normalized $\mathbf{g}(y|\lambda) = \lambda y$. Assume a gamma prior, $\mathbf{f}(\lambda|) = -(\alpha - 1)(\ln(\lambda) + \ln\beta - \ln(\alpha - 1) + 1) + \beta\lambda$. Then

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\begin{aligned}
(\mathbf{g} \cdot \mathbf{f})(y|) &= \min_{\lambda \in \mathbb{R}^+} [\mathbf{g}(y|\lambda) + \mathbf{f}(\lambda|)] \\
&= \min_{\lambda \in \mathbb{R}^+} [\lambda(y - \beta) - (\alpha - 1)(\ln(\lambda) + \ln\beta - \ln(\alpha - 1) + 1)] \\
&= \ln\left(\frac{y + \beta}{\beta}\right)(\alpha - 1)
\end{aligned}
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which is normalized since $\ln\left(\frac{0+\beta}{\beta}\right)(\alpha - 1) = 0$. This is the negative log of the Lomax distribution, but we have obtained its log-density through minimization by differentiation, rather than integration.

Example of morphisms and compositions from machine learning

State normalization under the min-plus semifield

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Outline

Defining the semifield homomorphism

Suppose, we have two arbitrary semifields $\mathbf{S} = (S, \oplus, \otimes, i_{\oplus}, i_{\otimes})$ and $\mathbf{S}' = (S', \oplus', \otimes', i_{\oplus'}, i_{\otimes'})$.

Definition

A function $h : S \to S'$ is a semifield homomorphism if for every $s_1, s_2 \in S$, the following equations hold

$$h(s_1 \oplus s_2) = h(s_1) \oplus' h(s_2)$$
$$h(s_1 \otimes s_2) = h(s_1) \otimes' h(s_2)$$
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Assume that $\mathbf{C}, \mathbf{C}'$ are affine semifield Markov categories over semifields $\mathbf{S} = (S, +, \times, 0, 1), \mathbf{S}' = (S', \oplus, \otimes, i_{\oplus}, i_{\otimes})$ respectively.

Theorem

Let $\mathbf{f} : X \to D(Y) \in \mathbf{C}$ and $\mathbf{f}' : X \to D(Y) \in \mathbf{C}'$. If there exists a semifield homomorphism $h : S \to S'$, then we can define a semifield transport functor $F : \mathbf{C} \to \mathbf{C}'$ is defined as the following;

1. *On objects $X \in \mathbf{C}$, $F(X) = X \in \mathbf{C}'$*
2. *On morphisms $\mathbf{f}, \mathbf{f}'$, $F(\mathbf{f})(y|x) = h(\mathbf{f}(y|x)) = \mathbf{f}'(y|x)$.*

Corollary

If there exists an isomorphism of semifields i.e. an inverse to the semifield homomorphism, then it is possible to construct an isomorphism of categories.

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An example transport functor

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Let $h(s) = -\frac{1}{a}\ln(s)$ for $a > 0$, mapping $[0,1] \to \mathbb{R}^{+} \cup \infty$. In this case, $h^{-1}(s') = \exp(-as')$ and we have

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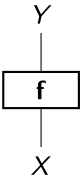

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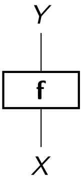

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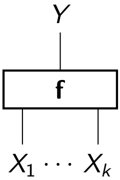

Representing DAGs as string diagrams

Suppose that we have a DAG that looks like

$P(ABCD) = P(A)P(B|D)P(D|A)P(C|B)$

Then we can represent it in string diagram notation as

- The morphism $\mathbf{a} : 1 \to D(A)$ contains the probability $P(A)$, $\mathbf{b} : A \to D(B)$ contains the probability $P(B|A)$,etc. The entire diagram is equal to a morphism $\mathbf{f} : 1 \to D(A \times B \times C \times D)$
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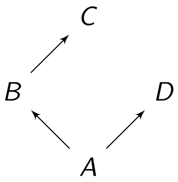

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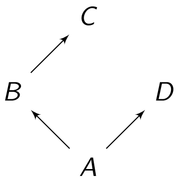

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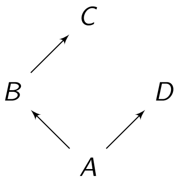

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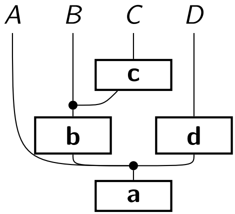

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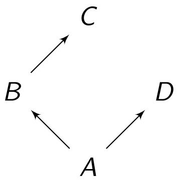

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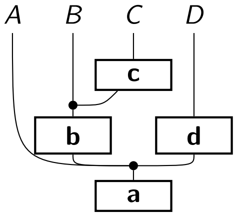

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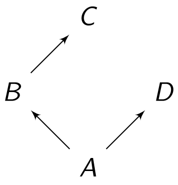

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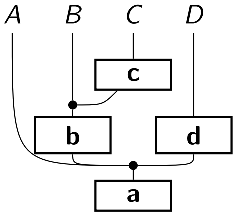

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Point-state cut functor

Definition

For any morphisms $\mathbf{f} : X_1 \times X_2 \times \cdots \times X_K \to D(Y)$, where $K \in \mathbb{N}$, the point-state cut functor $pcut_{\mathbf{f}}(\mathbf{f})$, acts in the following way

where $\mathbf{f} = f_0$ denotes a point-state morphism where f_0 is a fixed value, on morphisms $\mathbf{g} \neq \mathbf{f}$, $pcut_{\mathbf{f}}(\mathbf{g}) = \mathbf{g}$, and on objects X, $pcut_{\mathbf{f}}(X) = X$.

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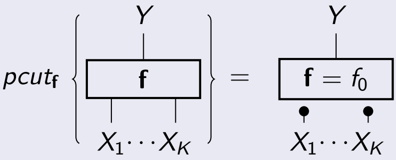

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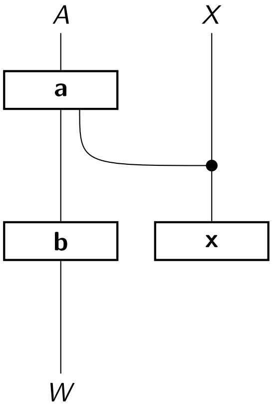

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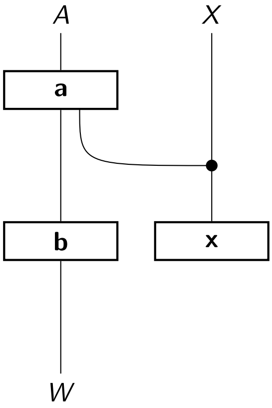

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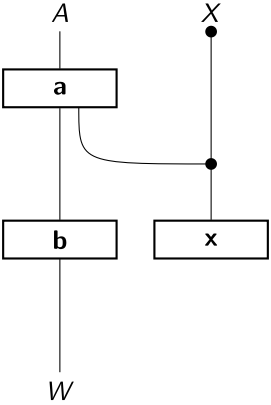

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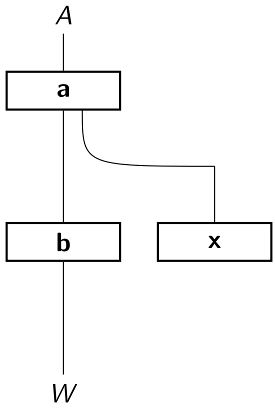

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The fixing morphism

Given a morphism $\mathbf{f}(a, x|w)$ then fixing operates with the following procedure;

- Marginalize out all the inputs to the morphism we want to fix on
- Replace the morphism with an identity wire
- Extend this new identity wire to become a new input to the entire diagram
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In the string diagram formalism, this is represented in the following example

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Suppose we have a morphism, $\mathbf{f}(a, x|w)$, the fixing morphism $\mathcal{F}_x(\mathbf{f})$, acts in the following way

Fixing in this example has the following effect, $\mathcal{F}_x(\mathbf{f}(a, x|w)) = \mathbf{f}(a|x, w)$. In some cases, x will just be marginalized out, and on a morphism $\mathbf{f}(a, y|w)$, fixing on x has the following effect $\mathcal{F}_x(\mathbf{f}(a, y|w)) = \mathbf{f}(a, y|w)$.

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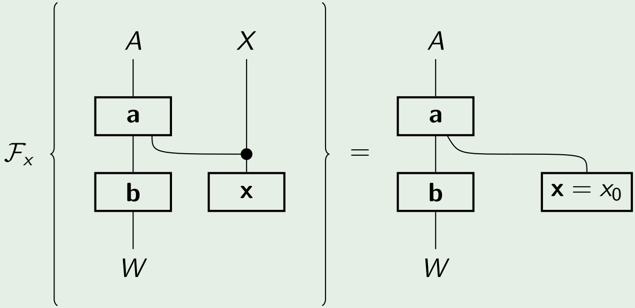

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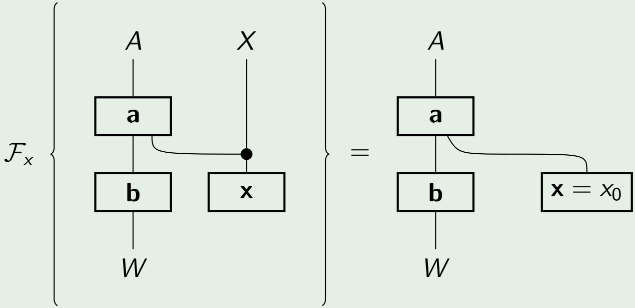

Fixing in this example has the following effect, $\mathcal{F}_x\,(\mathbf{f}\,(a, x|w)) = \mathbf{f}\,(a|x, w)$. In some cases, x will just be marginalized out, and on a morphism $\mathbf{f}\,(a, y|w)$, fixing on x has the following effect $\mathcal{F}_x\,(\mathbf{f}\,(a, y|w)) = \mathbf{f}\,(a, y|w)$.

Outline

Districts and kernels

String diagram perspective

- Districts are kernels (string diagrams) in which a set of unobserved common cause morphisms provides an input to other variables such as X, Y and this occurs transitively across all unobserved common cause morphisms.
- Here the district is $\mathbf{f}(x, y|z)$with internal kernel morphisms x, y, u.

Districts and kernels

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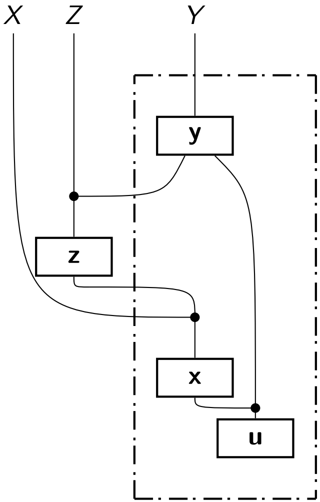

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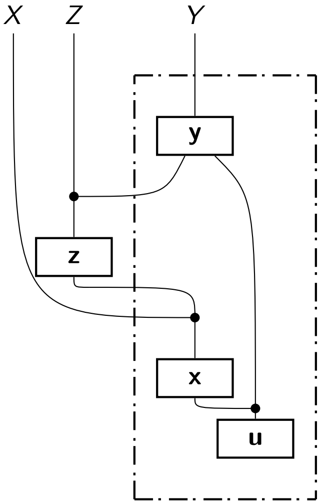

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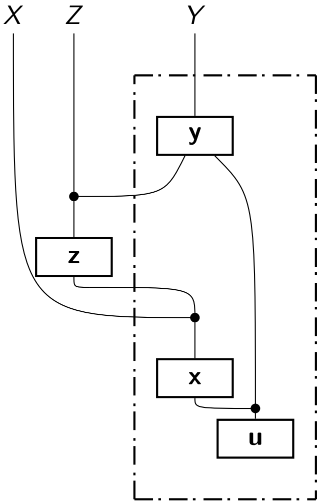

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Here we have the typical Back-door DAG in the string diagram formalism, in this example the morphism is given as $\mathbf{f}(c, x, y|)$,

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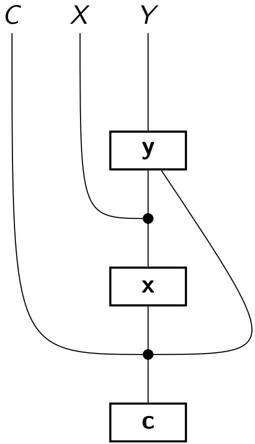

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When we apply $\mathcal{F}_x$ to the diagram it simulates intervention on x obtaining $\mathcal{F}_x(\mathbf{f}(c,x,y|)) = \mathbf{f}(c,y|x)$,

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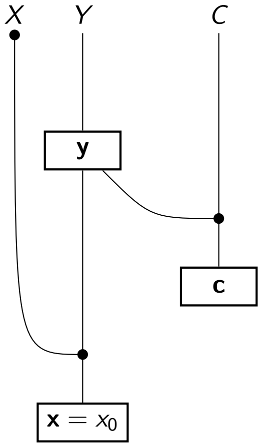

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After diagram simplification we obtain,

This is precisely $\mathbf{f}(c, y|x) = \mathbf{f}(c|)\,\mathbf{f}(y|x, c)$.

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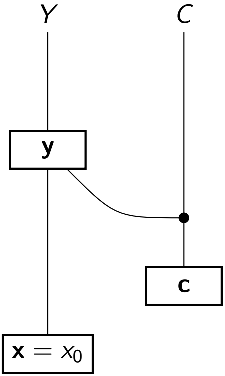

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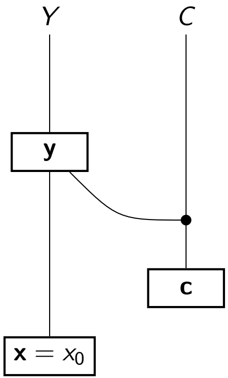

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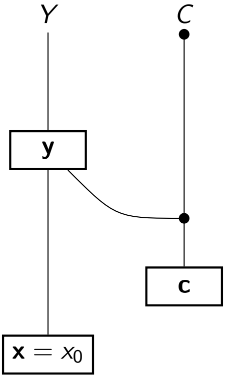

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Once we marginalize out c we obtain a diagram with the composite morphism $\mathbf{f}(c, y|x) = \sum_c \mathbf{f}(c|)\,\mathbf{f}(y|x, c)$ i.e. the back-door adjustment formula,

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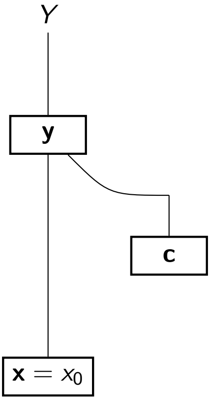

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Front-door adjustment through fixing

- In the front-door DAG, U is a hidden variable which influence both X and Y
- By latent projection U is replaced by a bidirected edge between X and Y
- In the string diagram representation we have the latent morphism $\mathbf{f}(u|)$ as an input to morphisms $\mathbf{f}(x|u)$ and $\mathbf{f}(y|z,u)$, but u itself is not exposed to the output.

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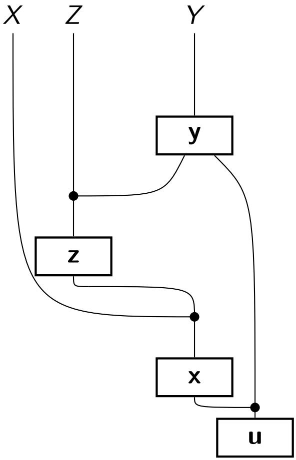

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We start with the the chain factored front-door diagram

We can identify z as a district and have a valid fixing sequence $\mathcal{F}_x\left(\mathcal{F}_y\left(\mathbf{f}\left(z|x\right)\right)\right)$.

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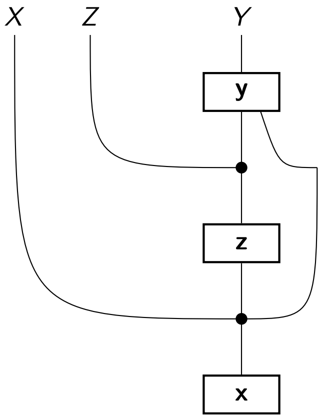

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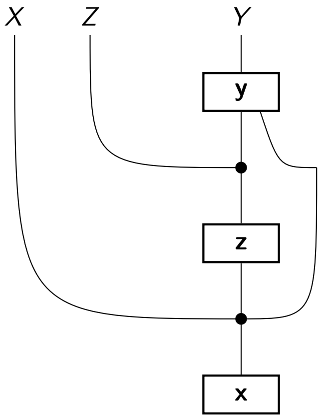

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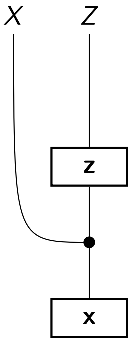

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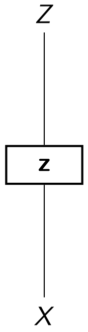

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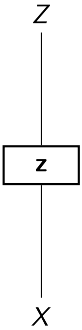

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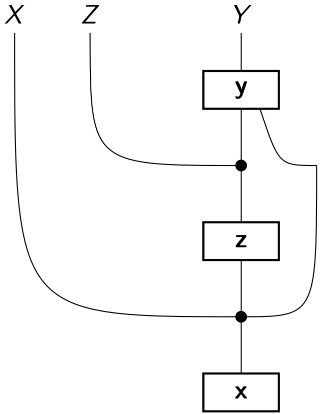

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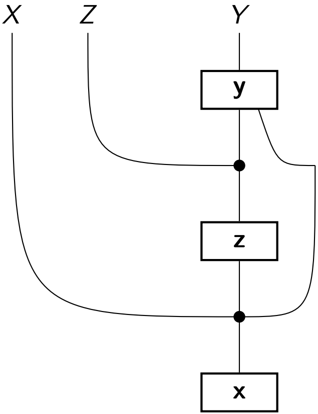

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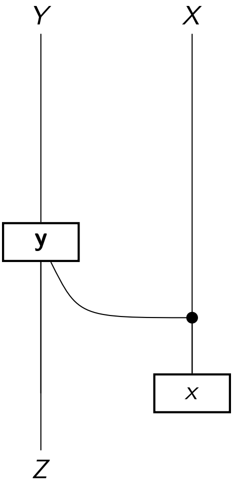

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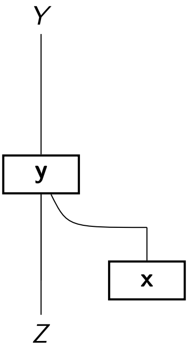

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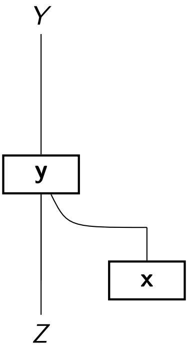

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Re-combining district kernel diagrams

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We can compose these two sequentially adhering to topological consistency.

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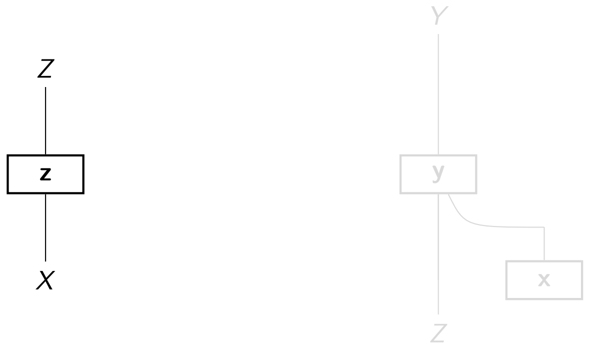

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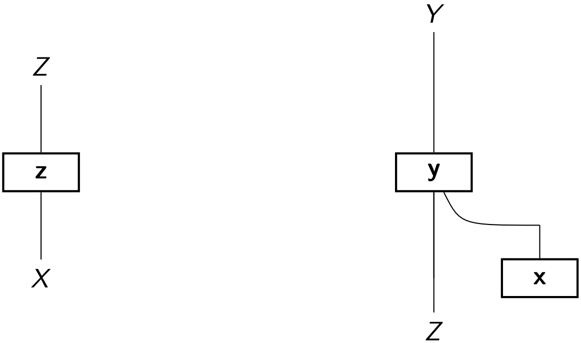

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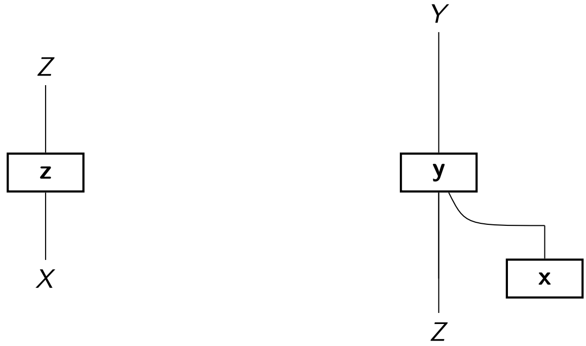

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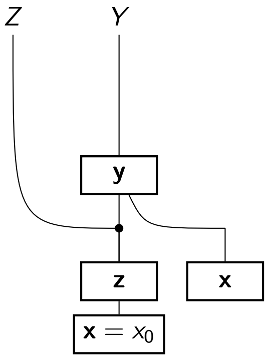

Summary

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- We have shown how it is possible to create formalism in which to conduct causal inference and machine learning together
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