(On the Power of) Knowledge Compilation in Causal Inference

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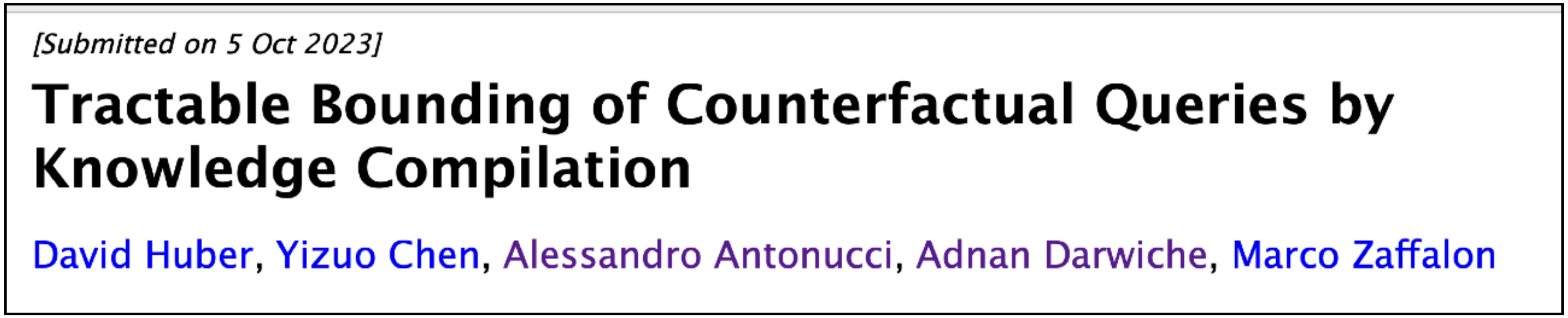
Workshop on Probabilistic Circuits and Logic - Simons Institute, Berkeley - Oct 17, 2023

What is this Talk about

"*Knowledge compilation has been successfully used to solve beyond NP problems, including some PP-complete and* $\textit{NP}^{\textit{PP}}$*-complete problems for Bayesian networks.*"

Solving $\textit{PP}^{\textit{PP}}$*-complete problems using knowledge compilation*,
Otzok, Choi, and Darwiche (KR, 2016)

6th Workshop on Tractable Probabilistic Modeling
Building Bridges

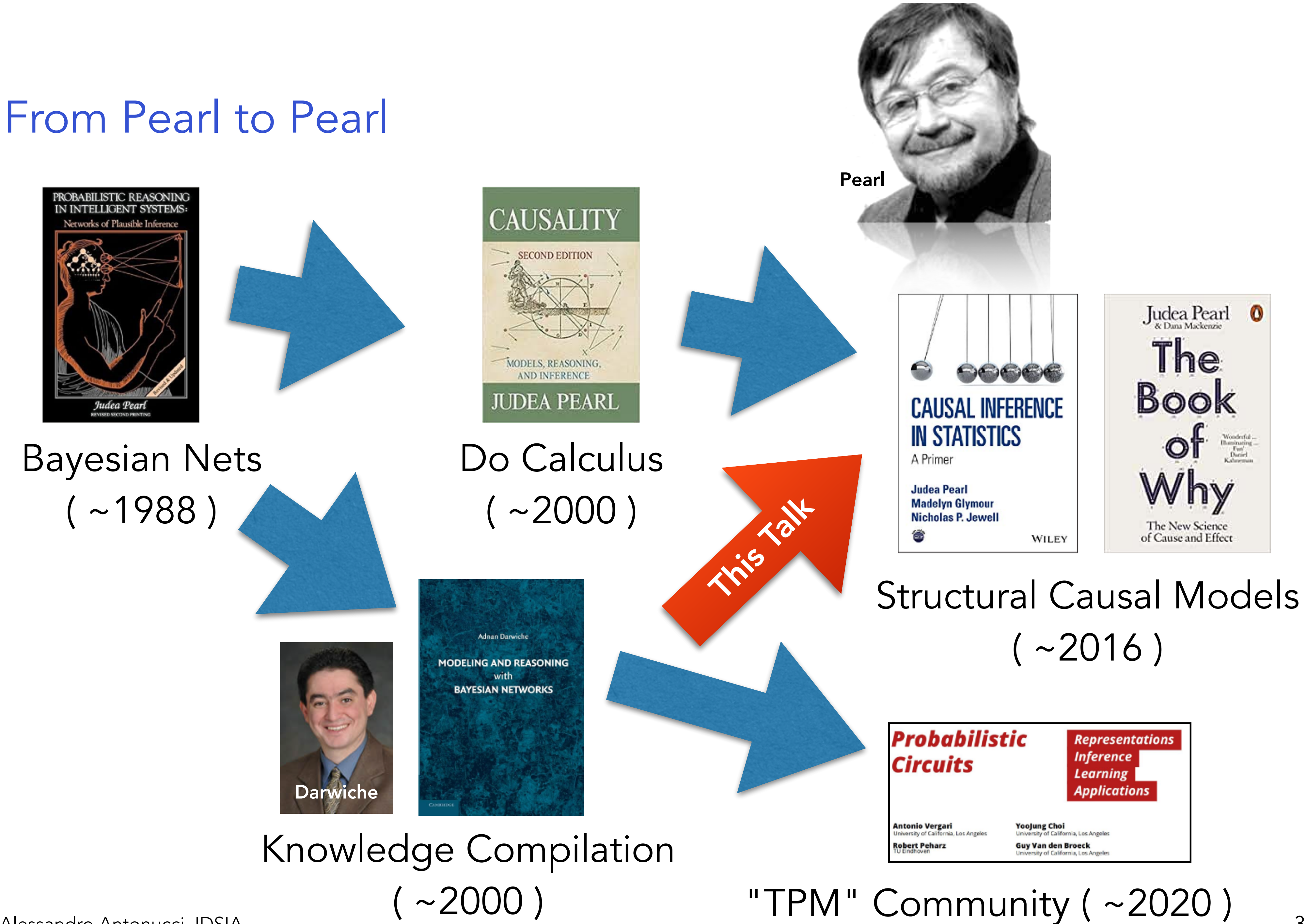


[Submitted on 5 Oct 2023]

Tractable Bounding of Counterfactual Queries by Knowledge Compilation

David Huber, Yizuo Chen, Alessandro Antonucci, Adnan Darwiche, Marco Zaffalon

From Pearl to Pearl


PROBABILISTIC REASONING IN INTELLIGENT SYSTEMS:
Networks of Plausible Inference
Judea Pearl
CAUSALITY
SECOND EDITION
MODELS, REASONING, AND INFERENCE
JUDEA PEARL
Pearl
CAUSAL INFERENCE IN STATISTICS
A Primer
Judea Pearl
Madelyn Glymour
Nicholas P. Jewell
WILEY
Judea Pearl
& Dana Mackenzie
The Book of Why
The New Science of Cause and Effect
This Talk
Darwiche
Adnan Darwiche
MODELING AND REASONING with BAYESIAN NETWORKS
Probabilistic Circuits
Representations
Inference
Learning
Applications
Antonio Vergari
University of California, Los Angeles
YooJung Choi
University of California, Los Angeles
Robert Peharz
TU Eindhoven
Guy Van den Broeck
University of California, Los Angeles

Bayesian Nets
(~1988)

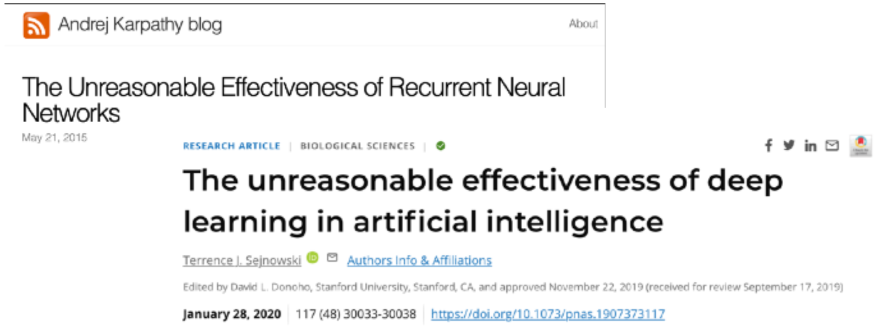
Do Calculus
(~2000)

Structural Causal Models
(~2016)

Knowledge Compilation
(~2000)

"TPM" Community (~2020)

(Science >) AI > Deep Learning



Andrej Karpathy blog About

The Unreasonable Effectiveness of Recurrent Neural Networks

May 21, 2015

RESEARCH ARTICLE | BIOLOGICAL SCIENCES |

The unreasonable effectiveness of deep learning in artificial intelligence

Terrence J. Sejnowski Authors Info & Affiliations

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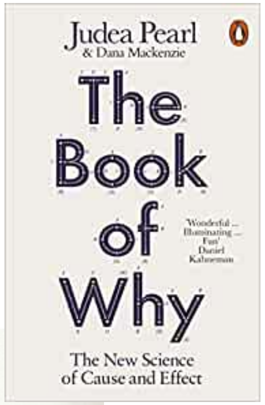
"Deep learning has instead given us machines with truly ***impressive abilities but no intelligence****.*

Pearl

The difference is profound and lies in the ***absence of a model of reality****."*



Judea Pearl
& Dana Mackenzie

The Book of Why

'Wonderful ... Illuminating ... Fun' Daniel Kahneman

The New Science of Cause and Effect

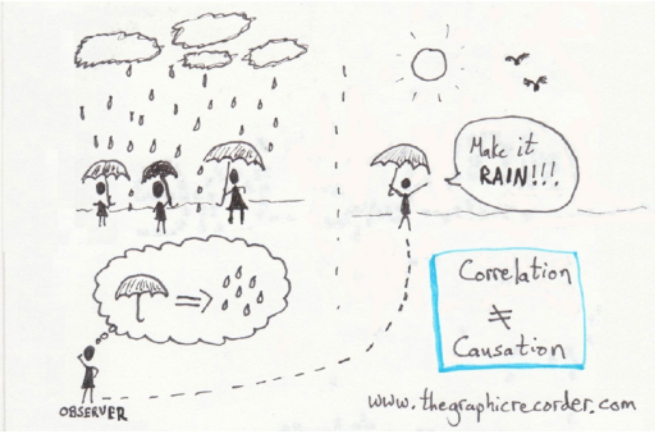
COMMUNICATIONS OF THE ACM

CACM.ACM.ORG 10/2018 VOL.61 NO.10

Human-Level Intelligence or Animal-Like Abilities?

Computing within Limits
Transient Electronics Take Shape
Q&A with Dina Katabi
Formally Verified Software in the Real World

Darwiche



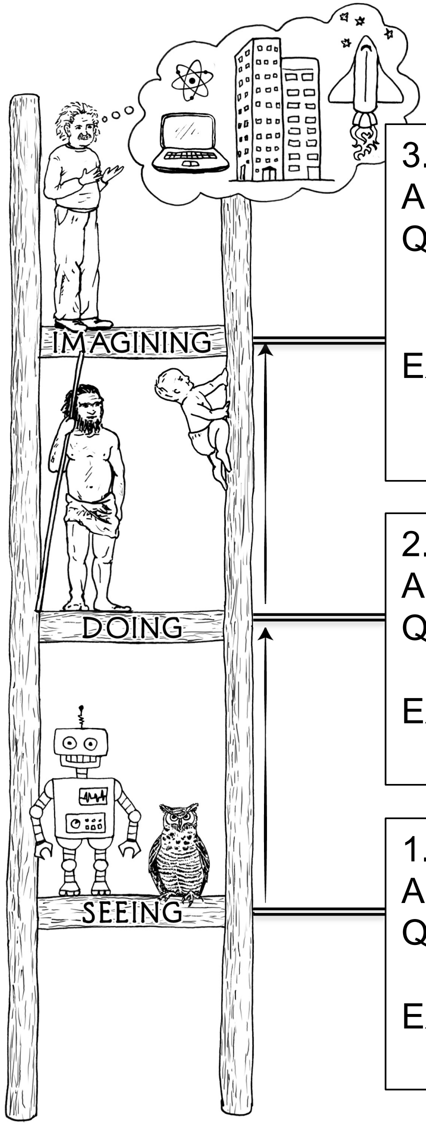
Pearl's Ladder of Causation and the Need for a Causal AI

3-LEVEL HIERARCHY

(Causal) AI?

RL

ML/DL



3. COUNTERFACTUALS
ACTIVITY: Imagining, Retrospection, Understanding
QUESTIONS: *What if I had done . . . ? Why?*
(Was it X that caused Y? What if X had not occurred? What if I had acted differently?)
EXAMPLES: Was it the aspirin that stopped my headache?
Would Kennedy be alive if Oswald had not killed him? What if I had not smoked the last 2 years?

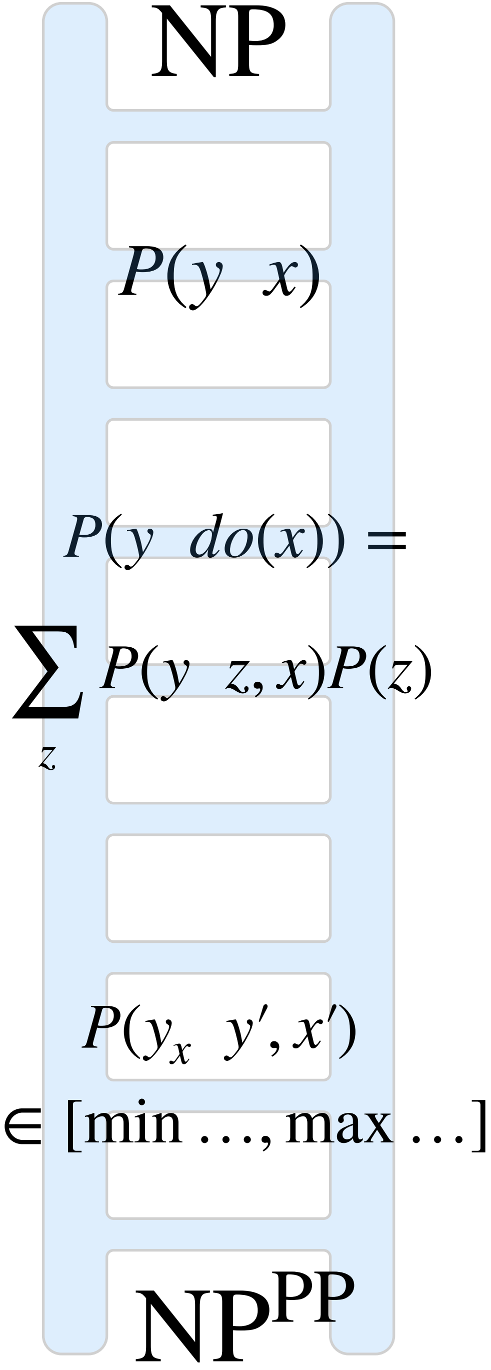
2. INTERVENTION
ACTIVITY: Doing, Intervening
QUESTIONS: *What if I do . . . ? How?*
(What would Y be if I do X?)
EXAMPLES: If I take aspirin, will my headache be cured?
What if we ban cigarettes?

1. ASSOCIATION
ACTIVITY: Seeing, Observing
QUESTIONS: *What if I see . . . ?*
(How would seeing X change my belief in Y?)
EXAMPLES: What does a symptom tell me about a disease?
What does a survey tell us about the election results?

Source: The Book of Why, Pearl & Mc Kenzie

A Ladder for (PGM) Inference?

- Answering an **observational** query?
  Single PGM query in the empirical model
- (Identifiable) **interventional** query?
  - **Do-calculus** and queries by auxiliary PGM inferences in the empirical model
  - Single EM on the SCM with latent variables + PGM inference (Dechter, 2023)
- **Counterfactual** queries suffer partial identifiability (**bounds** only)
  - Credal nets (Zaffalon & Antonucci, 2020)
  - Multiple EM runs (Zaffalon & Antonucci, 2021)
  - Sampling (Bareinboim, 2022)
  - Polynomial programs (Shpitser, 2023)
  - Multiple EM + KG (this talk)



NP

$P(y\ \ x)$

$P(y\ \ do(x)) =$

$\sum_{z} P(y\ \ z, x)P(z)$

$P(y_x\ \ y', x')$

$\in [\min \ldots, \max \ldots]$

$\mathrm{NP}^{\mathrm{PP}}$

Structural Causal Models (Univariate)

- Manifest **endogenous** variable X
- Observations $\mathscr{D}$ available
- From $\mathscr{D}$ statistical learning of $P(X)$

Boolean X

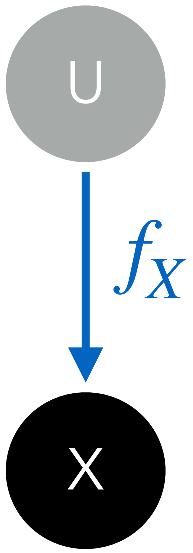
$P(X=0)=p$

Structural Causal Models (Univariate)

- Manifest **endogenous** variable X
- Observations $\mathscr{D}$ available
- From $\mathscr{D}$ statistical learning of $P(X)$
- A latent **exogenous** variable U
- U determines X (**structural equation** f_X)
- $P(U)$ induces (a single) $P(X)$

$$P(x) = \sum_x P(x \quad u)P(u) = \sum_u \delta_{f(u),x} P(u)$$

$U \in \{0,1,2,3\}$



$f_X(U=0)=0$

$f_X(U=1)=0$

$f_X(U=2)=1$

$f_X(U=3)=1$

Boolean X

$P(X=0)=p$

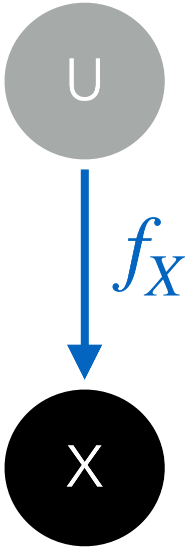
Structural Causal Models (Univariate)

$K(U) = \{P(U) : P(U=0) + P(U=1) = p\}$

$$P(U) = \left[\frac{p}{2}, \frac{p}{2}, \frac{1-p}{2}, \frac{1-p}{2}\right]$$

$U \in \{0,1,2,3\}$

- Manifest **endogenous** variable X
- Observations $\mathscr{D}$ available
- From $\mathscr{D}$ statistical learning of $P(X)$
- A latent **exogenous** variable U
- U determines X (**structural equation** f_X)
- $P(U)$ induces (a single) $P(X)$
  $$P(x) = \sum_x P(x \ \ u)P(u) = \sum_u \delta_{f(u),x} P(u)$$
- $P(X)$ to $P(U)$? Multiple consistent $P(U)$'s
- Bounds? Query has different values for the different consistent $P(U)$!



$f_X(U=0) = 0$

$f_X(U=1) = 0$

$f_X(U=2) = 1$

$f_X(U=3) = 1$

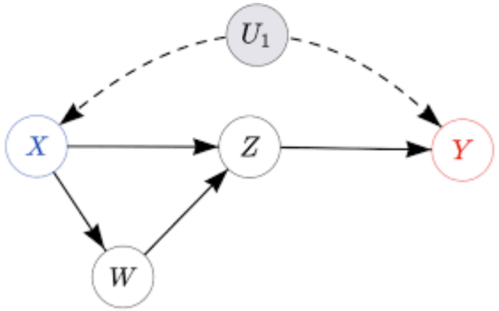
Boolean X

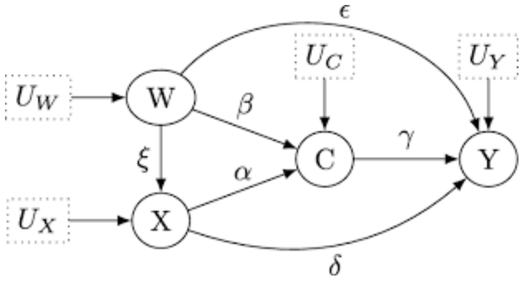
$P(X=0) = p$

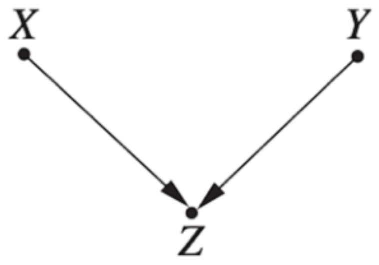
Structural Causal Models

- $\mathbf{X} := (X_1, \ldots, X_n)$ (endogenous variables)
- $\mathbf{U} := (U_1, \ldots, U_m)$ (exogenous variables)
- Directed graph $\mathscr{G}$ assumed to be semi-Markovian = root in $\mathbf{U}$, non-root in $\mathbf{X}$

- Equation $X = f_X(\mathrm{Pa}_X)$ for each $X \in \mathbf{X}$
  - Exogenous states $\mathbf{U} = \mathbf{u}$ determine endogenous states $\mathbf{X} = \mathbf{x}$
- Marginal $P(U)$ for each $U \in \mathbf{U}$
  - Exogenous distribution distribution $P(\mathbf{U})$ induces endogenous distribution $P(\mathbf{X})$







$U = \{X, Y\}, \quad V = \{Z\}, \quad F = \{f_Z\}$

$f_Z : Z = 2X + 3Y$

SCMs as BNs?

- **An SCM is a BN** with CPTs $P(X \ \ \mathrm{Pa}_X) = \delta_{X,f_X(\mathrm{Pa}_X)}$

$$P(\mathbf{x},\mathbf{u}) = \prod_{U \in \mathbf{U}} P(u) \prod_{X \in \mathbf{X}} \delta_{f_X(\mathrm{pa})_X,x}$$

- We need:
  - Causal Graph (= Exogenous Confounders)
  - Structural Equations (= Endogenous CPTs)
  - Exogenous Marginals

FSCM = Fully Specified

- Often we only have:
  - Causal Graph
  - Endogenous Data
  - Structural Equations? "Canonical" specification

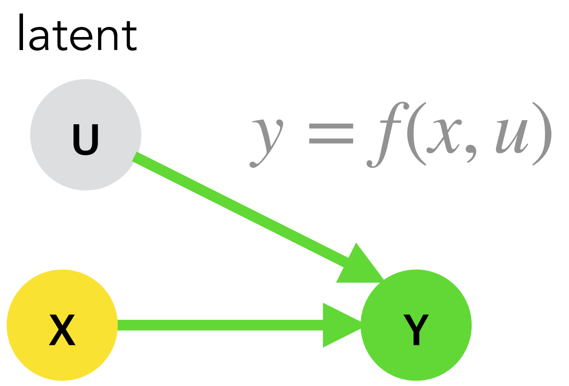
PSCM = Partially Specified

Canonical Specification of Structural Equations

- Structural equations from $\mathscr{G}$?
- $y = f(x, u)$? Canonical? U indexing all deterministic mechanisms btw X and Y
- With Boolean parent & child?
- $U \quad = 4$
- In general, exponential size:

$$U \quad = \quad Y \quad ^{\prod_{X \in \mathrm{Pa}_Y} \quad X}$$

- Even larger cardinality if Y has more than an exogenous parent



ex. disease and test outcome

$$P(Y \quad X, U)$$

	X=0	X=1	X=0	X=1	X=0	X=1	X=0	X=1
Y=0	1	1	1	0	0	1	0	0
Y=1	0	0	0	1	1	0	1	1
	U=0		U=1		U=2		U=3	
	$Y = 0$		$Y = X$		$Y = \neg X$		$Y = 1$	

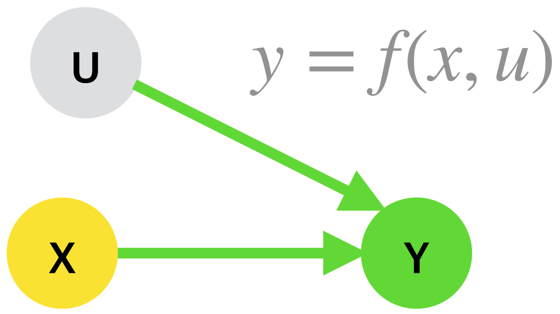
Canonical Specification of Structural Equations

- Structural equations from $\mathscr{G}$?
- $y = f(x, u)$? Canonical? U indexing all deterministic mechanisms btw X and Y
- With Boolean parent & child?
- $U \quad = 4$
- In general, exponential size:

$$U \quad = \quad Y^{\prod_{X \in \mathrm{Pa}_Y} \quad \mathrm{X}}$$

- Even larger cardinality if Y has more than an exogenous parent
- Non-canonical? Domain knowledge (ex. $Y = 1$ and $Y = \neg X$ impossible)

latent



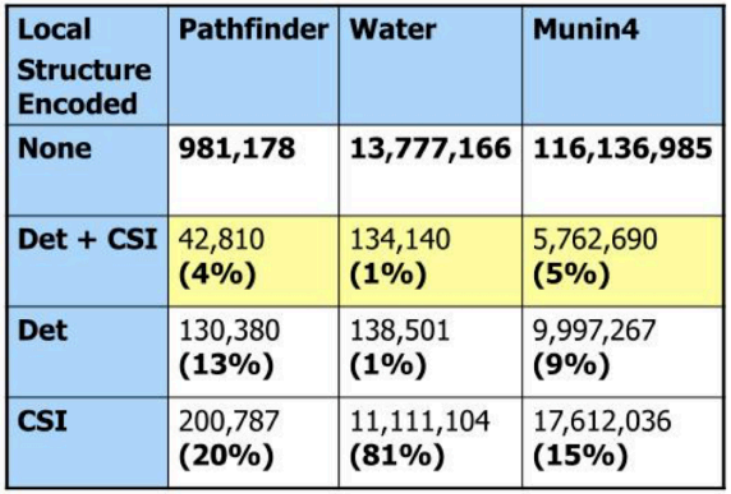
ex. disease and test outcome

$$P(Y \quad X, U)$$

	X=0	X=1	X=0	X=1	X=0	X=1	X=0	X=1
Y=0	1	1	1	0	[redacted]	[redacted]	[redacted]	[redacted]
Y=1	0	0	0	1	[redacted]	[redacted]	[redacted]	[redacted]
	U=0		U=1		U=2		U=3	
	$Y = 0$		$Y = X$		$Y = \neg X$		$Y = 1$	

Inference in FSCMs

- BN inference is $O(2^{\text{treewidth}})$, faster with:
  - **c**ontext-**s**pecific **i**ndependence
  - **det**erminism
- FSCM = BN + determinism in CPTs
  - Compilation to tractable circuits with FSCMs of high tw (>100)
  - Causal treewidth ≤ treewidth inference $O(2^{\text{causal treewidth}})$
- Operational characterisation (Darwiche, 2022)
- Counterfactuals? ctw x (# of worlds)
- Standard compilers (ex. ACE) not specialized to FSCMs



Local Structure Encoded	Pathfinder	Water	Munin4
None	981,178	13,777,166	116,136,985
Det + CSI	42,810 (4%)	134,140 (1%)	5,762,690 (5%)
Det	130,380 (13%)	138,501 (1%)	9,997,267 (9%)
CSI	200,787 (20%)	11,111,104 (81%)	17,612,036 (15%)

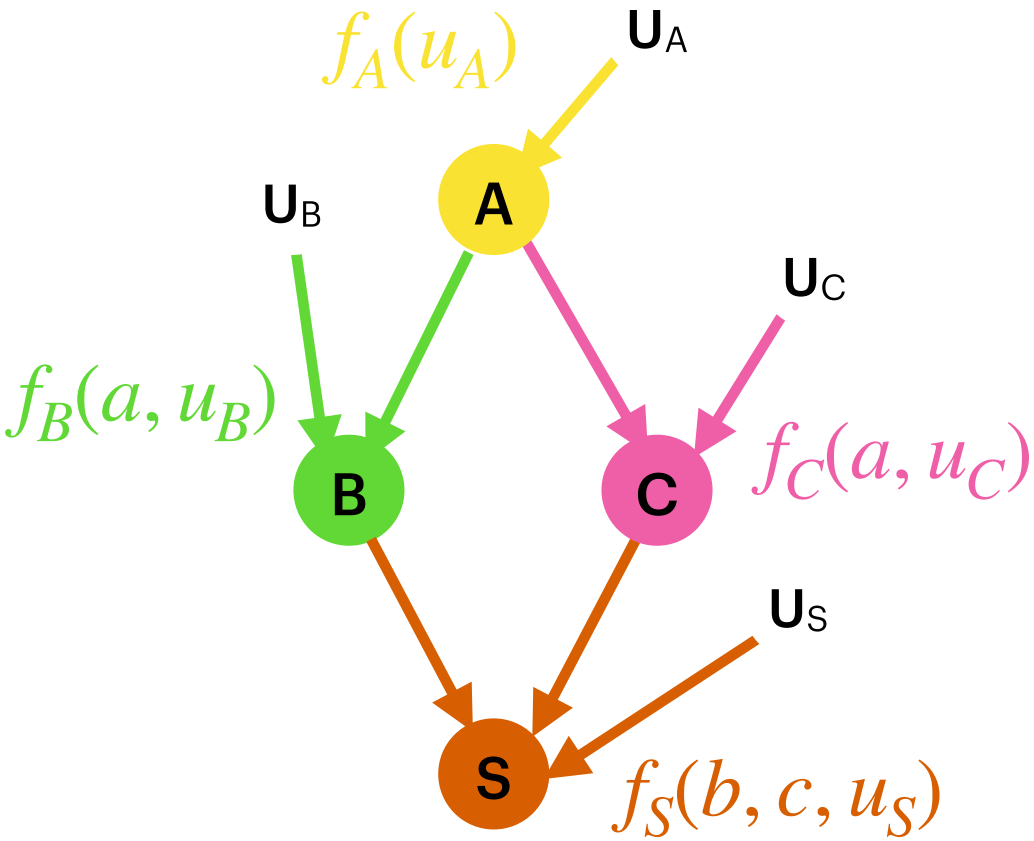
Inference in PSCMs

- More challenging than FSCM inference
- Identifiable queries?
  - Do-calculus = inference in the empirical BN
- Non-identifiable?
  - Bound computation
  - Equivalent to inference in a **credal net** (i.e., bounds wrt iterated BN inference)
  - NP^{PP} task (Zaffalon and Antonucci, 2023)
- PSCM = Collection of compatible FSCMs
- Let's write the compatibility constraints!

Credal Net Mapping

- Find the exogenous marginals?

  $P(U_A)P(U_B)P(U_C)P(U_S)$
- **Endogenous** (= with $\mathscr{D}$) **consistency**
- This induces global non-linear (so-called Verma) constraints
- Let's make the constraints local and linear by marginalisation and conditioning



$$\sum_{u_A,u_B,u_C,u_D}\left[\overset{\text{Unknown}}{p(u_A)}\cdot\delta_{a,f_A(u_A)}\cdot\overset{\text{Unknown}}{p(u_B)}\cdot\delta_{b,f_B(a,u_B)}\cdot\overset{\text{Unknown}}{p(u_C)}\cdot\delta_{c,f_C(a,u_c)}\cdot\overset{\text{Unknown}}{p(u_S)}\cdot\delta_{s,f_S(b,c,u_S)}\right]=\overset{\text{Empirical, known}}{\tilde{p}(a,b,c,s)}$$

Credal Net Mapping (con't)

$$\sum_{u_A,u_B,u_C,u_D}\left[p(u_A)\cdot\delta_{a,f_A(u_A)}\cdot p(u_B)\cdot\delta_{b,f_B(a,u_B)}\cdot p(u_C)\cdot\delta_{c,f_C(a,u_C)}\cdot p(u_S)\cdot\delta_{s,f_S(b,c,u_S)}\right]=\tilde{p}(a,b,c,s)$$

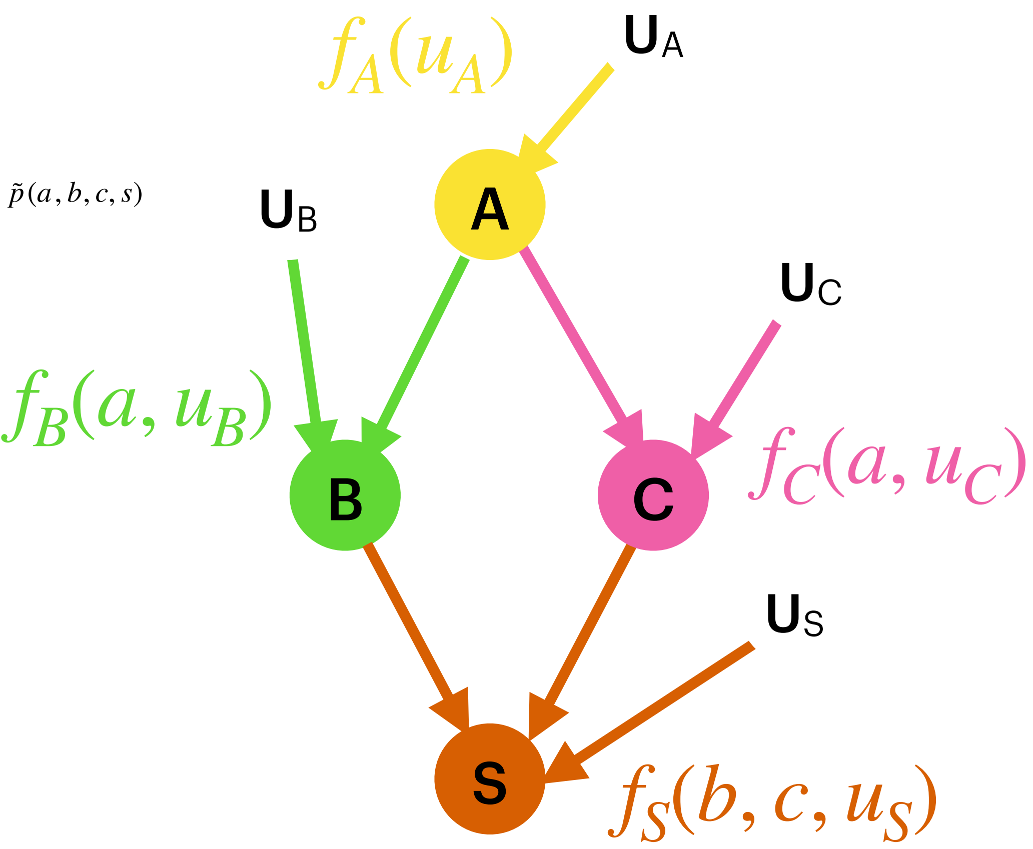
⬇

$$P(a)=\sum_{u_A}P(a\;\;u_A)\cdot P(u_A)$$

$$P(b\;\;a)=\sum_{u_B}P(b\;\;a,u_B)\cdot P(u_B)$$

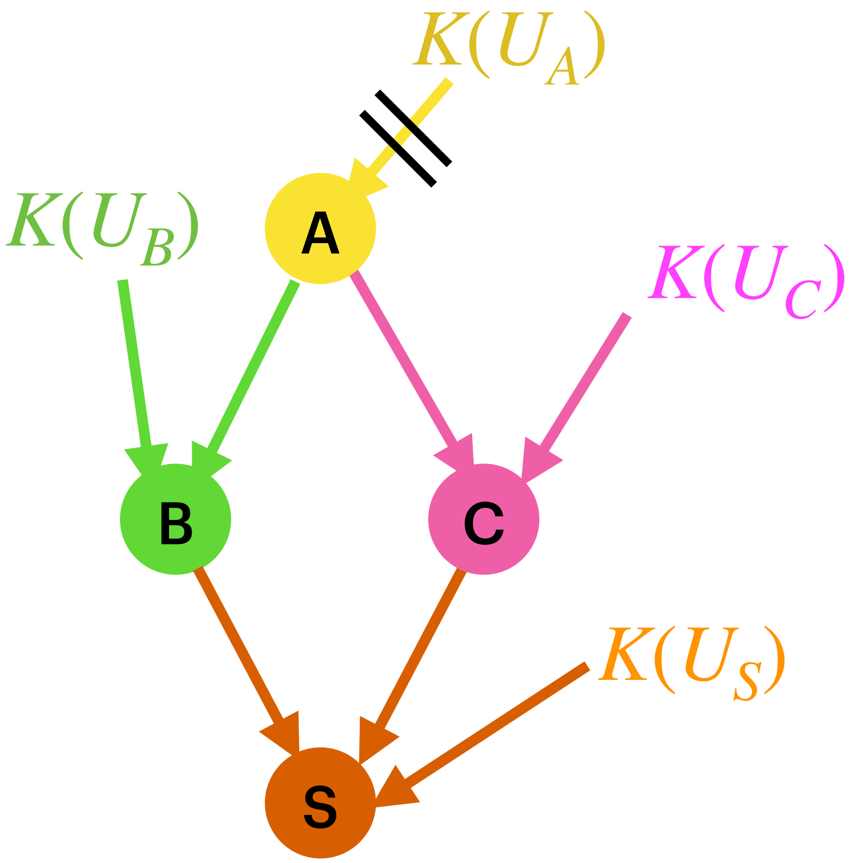
$$P(c\;\;a)=\sum_{u_C}P(c\;\;a,u_C)\cdot P(u_C)$$

$$P(s\;\;b,c)=\sum_{u_S}P(s\;\;b,c,u_S)\cdot P(u_S)$$



- Linear constraints on marginal exogenous probabilities leading to the (credal) set specification $K(U_A)$, $K(U_B)$, $K(U_C)$, $K(U_S)$
- Structural equations (= endogenous CPTS) remain unaffected

Causal Inference by Credal Nets



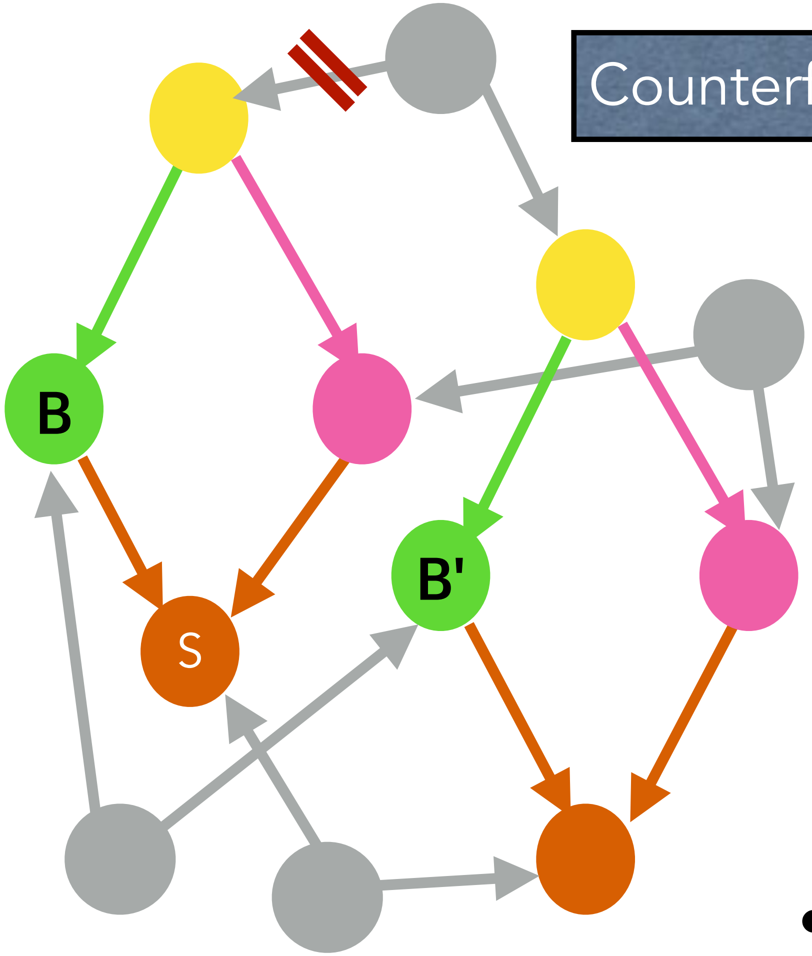
$$P(B\ \ \mathrm{do}(\bar{a})) \in [\underline{P}^{'}(B\ \ \bar{a}), \overline{P}'(B\ \ \bar{a})]$$

Interventional query

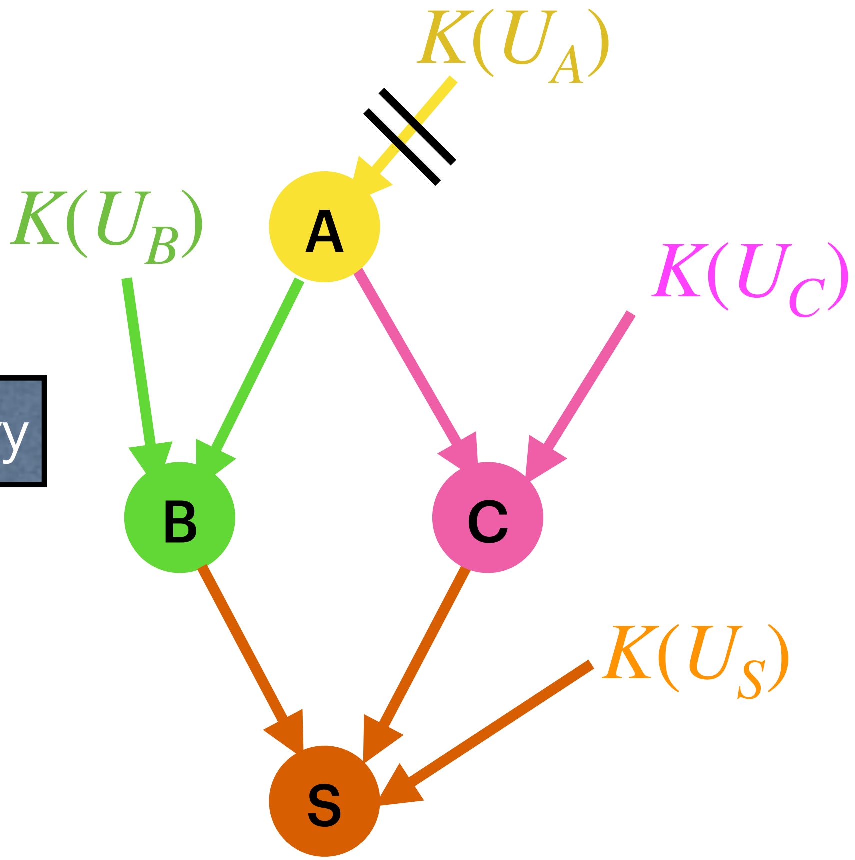
- Identifiable? $\underline{P} = \overline{P}$

Causal Inference by Credal Nets

$P(S_b\ \ \overline{b}) \in [\underline{P}(S\ \ b,\overline{b}'),\overline{P}(S\ \ b,\overline{b}')]$



Counterfactual query



$P(B\ \ \mathrm{do}(\overline{a})) \in [\underline{P}^{'}(B\ \ \overline{a}),\overline{P}'(B\ \ \overline{a})]$

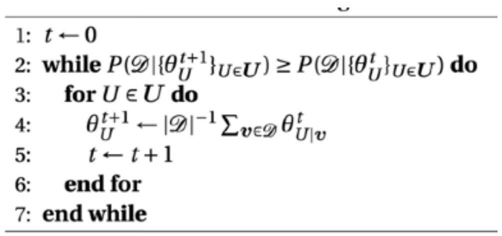
Interventional query

- Identifiable? $\underline{P} = \overline{P}$

Causal EM (Zaffalon & Antonucci, 2021)

- CN mapping suffers in models with multiple exogenous parents
- Exogenous variables are always missing (MAR, asystematic, way)
- Expectation Maximisation (Dempster, 1977)
  - Random initialisation of P(U)
  - E-step: Missing data completion by expected (fractional) counts
  - M-step: "completed" data to retrain P(U)
  - Iterate until convergence
- EM goes to a (local/global) max of log-lik

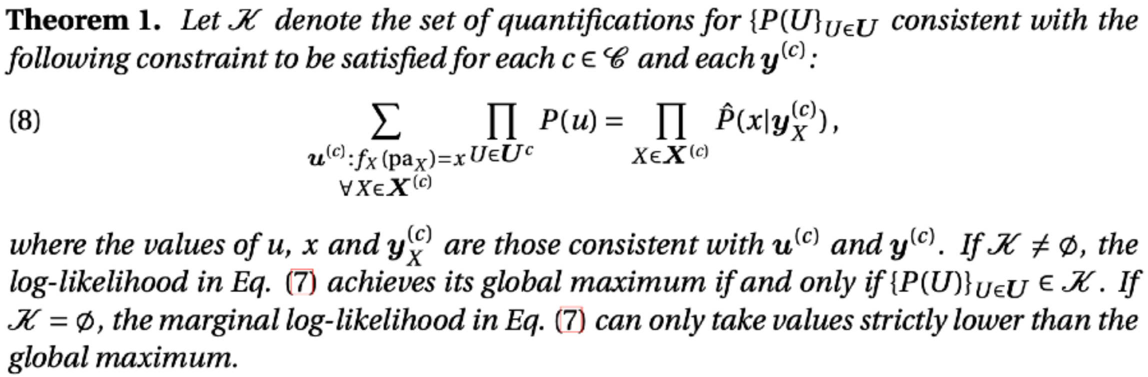
U1	U2	X1	X2	n
*	*	0	0	…
*	*	0	1	…
*	*	1	0	…
*	*	1	1	…



```
$t \leftarrow 0$
while $P(\mathscr{D}|\{\theta_U^{t+1}\}_{U\in\boldsymbol{U}}) \geq P(\mathscr{D}|\{\theta_U^{t}\}_{U\in\boldsymbol{U}})$ do
    for $U \in \boldsymbol{U}$ do
        $\theta_U^{t+1} \leftarrow |\mathscr{D}|^{-1} \sum_{\boldsymbol{v}\in\mathscr{D}} \theta_{U|\boldsymbol{v}}^{t}$
        $t \leftarrow t+1$
    end for
end while
```

Causal EM: Getting an Inner Approximation of the Bounds

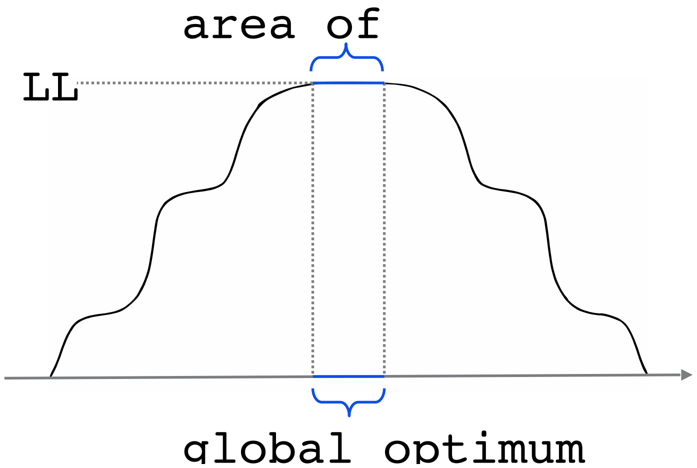
- Causal EM converge to global maximum (that we know) if and only if the corresponding $P(U)$ belongs to credal set $K(U)$
- We sample initialisations, to sample $K(U)$
- For each sample we obtain an inner point



Theorem 1. *Let $\mathcal{K}$ denote the set of quantifications for $\{P(U)\}_{U\in\boldsymbol{U}}$ consistent with the following constraint to be satisfied for each $c \in \mathscr{C}$ and each $\boldsymbol{y}^{(c)}$:*

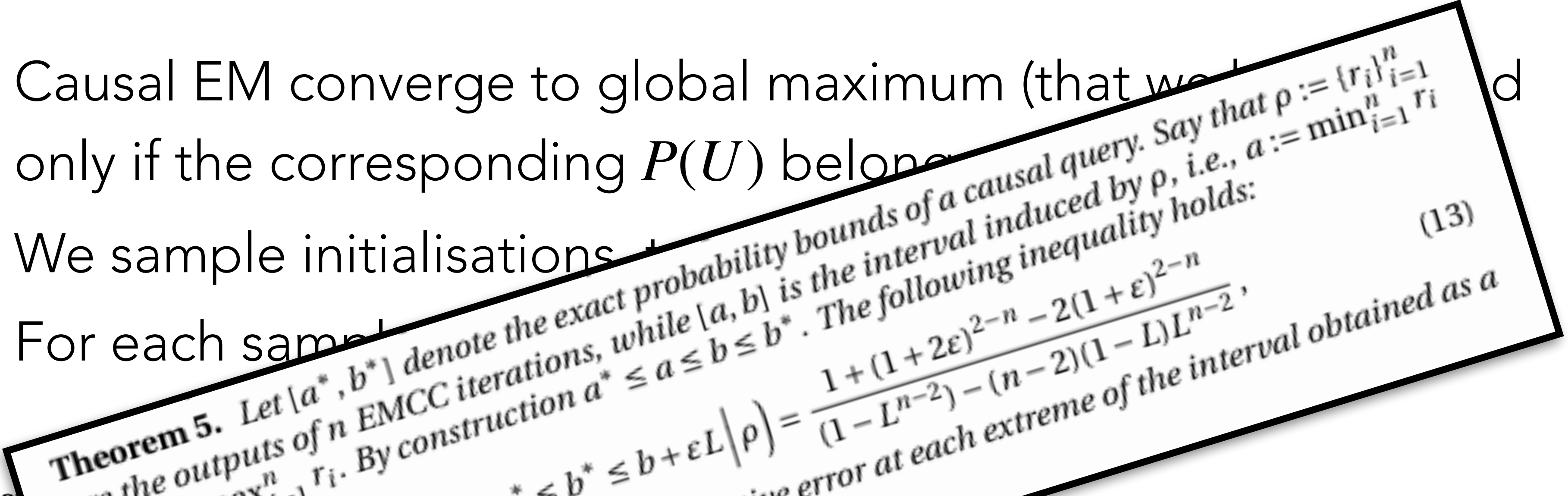
$$\sum_{\substack{\boldsymbol{u}^{(c)}: f_X(\mathrm{pa}_X)=x \\ \forall X\in\boldsymbol{X}^{(c)}}} \prod_{U\in\boldsymbol{U}^c} P(u) = \prod_{X\in\boldsymbol{X}^{(c)}} \hat{P}(x|\boldsymbol{y}_X^{(c)}), \tag{8}$$

where the values of u, x and $\boldsymbol{y}_X^{(c)}$ are those consistent with $\boldsymbol{u}^{(c)}$ and $\boldsymbol{y}^{(c)}$. If $\mathcal{K} \neq \emptyset$, the log-likelihood in Eq. (7) achieves its global maximum if and only if $\{P(U)\}_{U\in\boldsymbol{U}} \in \mathcal{K}$. If $\mathcal{K} = \emptyset$, the marginal log-likelihood in Eq. (7) can only take values strictly lower than the global maximum.



Causal EM: Getting an Inner Approximation of the Bounds

- Causal EM converge to global maximum (that we d only if the corresponding $P(U)$ belong
- We sample initialisations
- For each samp



Theorem 5. *Let $[a^*, b^*]$ denote the exact probability bounds of a causal query. Say that $\rho := \{r_i\}_{i=1}^n$ are the outputs of n EMCC iterations, while $[a, b]$ is the interval induced by ρ, i.e., $a := \min_{i=1}^n r_i$ and $b := \max_{i=1}^n r_i$. By construction $a^* \leq a \leq b \leq b^*$. The following inequality holds:*

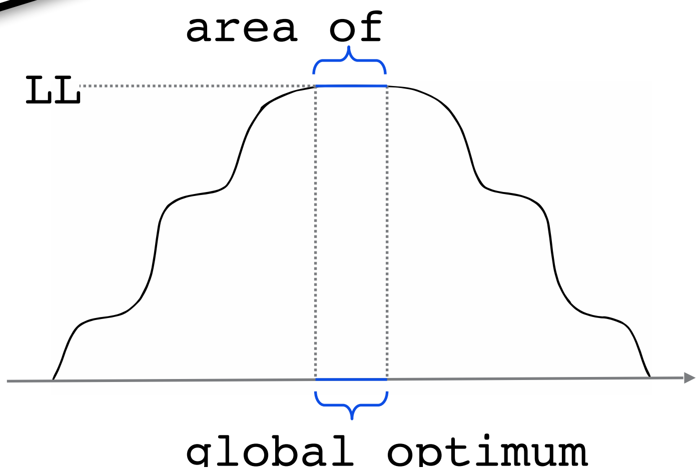
$$P\left(a - \varepsilon L \leq a^* \leq b^* \leq b + \varepsilon L \,\middle|\, \rho\right) = \frac{1 + (1+2\varepsilon)^{2-n} - 2(1+\varepsilon)^{2-n}}{(1 - L^{n-2}) - (n-2)(1-L)L^{n-2}}, \qquad (13)$$

where $L := (b - a)$ and $\varepsilon := \delta/(2L)$ is the relative error at each extreme of the interval obtained as a function of the absolute allowed error $\delta \in (0, L)$.

Theo *follow*

(8)

where the ose consistent with $\mathbf{u}^{(c)}$ and $\mathbf{y}^{(c)}$. If $\mathcal{K} \neq \emptyset$, the log-likeliho ves its global maximum if and only if $\{P(U)\}_{U \in \mathbf{U}} \in \mathcal{K}$. If $\mathcal{K} = \emptyset$, the m og-likelihood in Eq. (7) can only take values strictly lower than the global maximum.



Causal EM: Getting an Inner Approximation of the Bounds

- Causal EM converge to global maximum (that w d only if the corresponding $P(U)$ belon
- We sample initialisations
- For each samp

Theorem 5. *Let $[a^*, b^*]$ denote the exact probability bounds of a causal query. Say that $\rho := \{r_i\}_{i=1}^n$ are the outputs of n EMCC iterations, while $[a, b]$ is the interval induced by ρ, i.e., $a := \min_{i=1}^n r_i$ and $b := \max_{i=1}^n r_i$. By construction $a^* \le a \le b \le b^*$. The following inequality holds:*

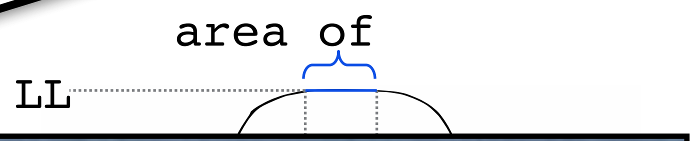
$$P\left(a-\varepsilon L \le a^* \le b^* \le b+\varepsilon L \middle| \rho\right) = \frac{1+(1+2\varepsilon)^{2-n}-2(1+\varepsilon)^{2-n}}{(1-L^{n-2})-(n-2)(1-L)L^{n-2}}, \quad (13)$$

where $L := (b-a)$ and $\varepsilon := \delta/(2L)$ is the relative error at each extreme of the interval obtained as a function of the absolute allowed error $\delta \in (0, L)$.

Theo *follow*

(8)

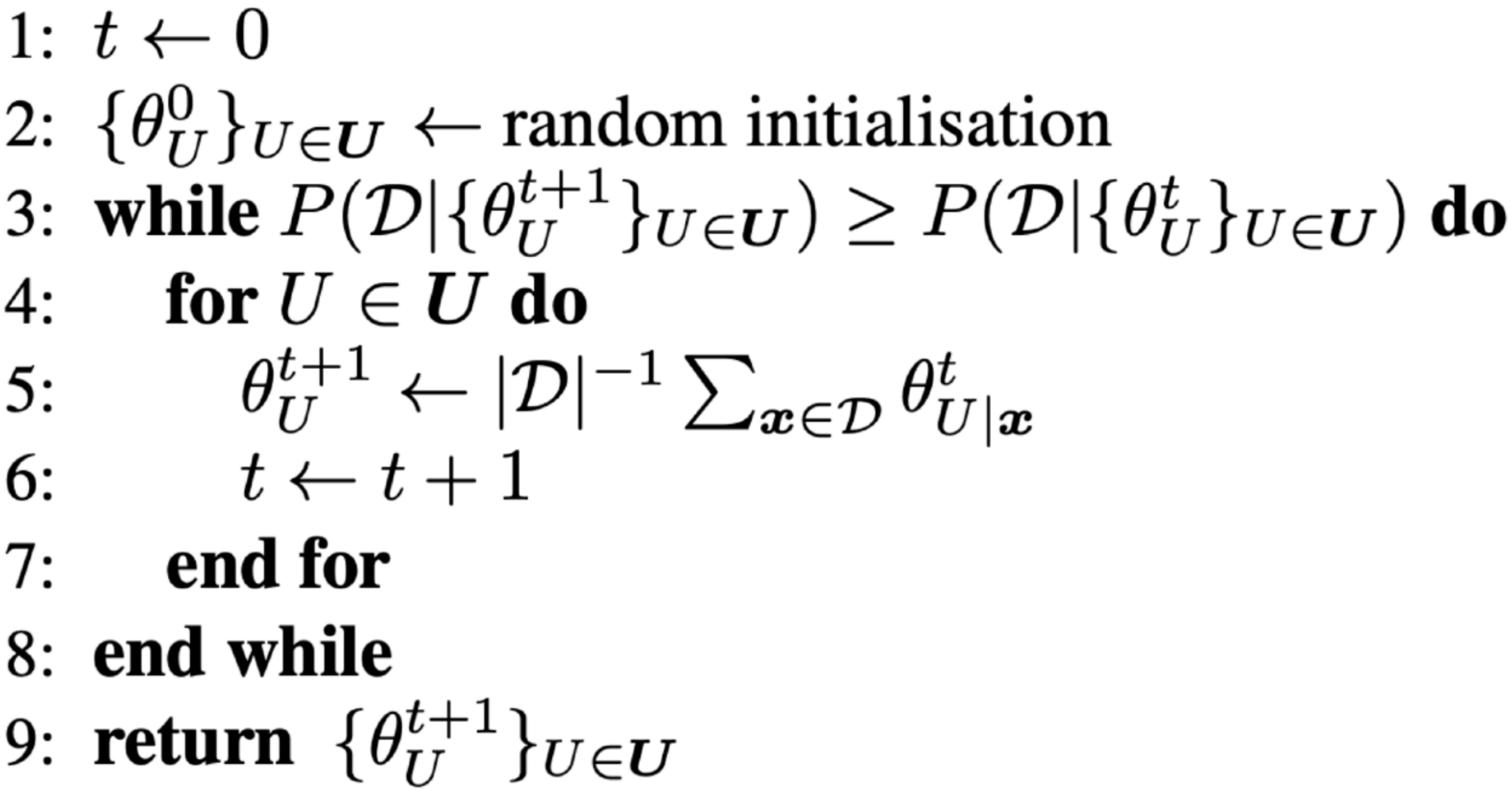
where the *those consistent* *log-likeliho* *ves its global maximum* *$\mathcal{K} = \emptyset$, the n* *log-likelihood in Eq. (7) can only* *global maximum.*



20 EM runs to get close to the actual bounds with 95% credibility

For identifiable queries 9 runs to be sure with 99% credibility

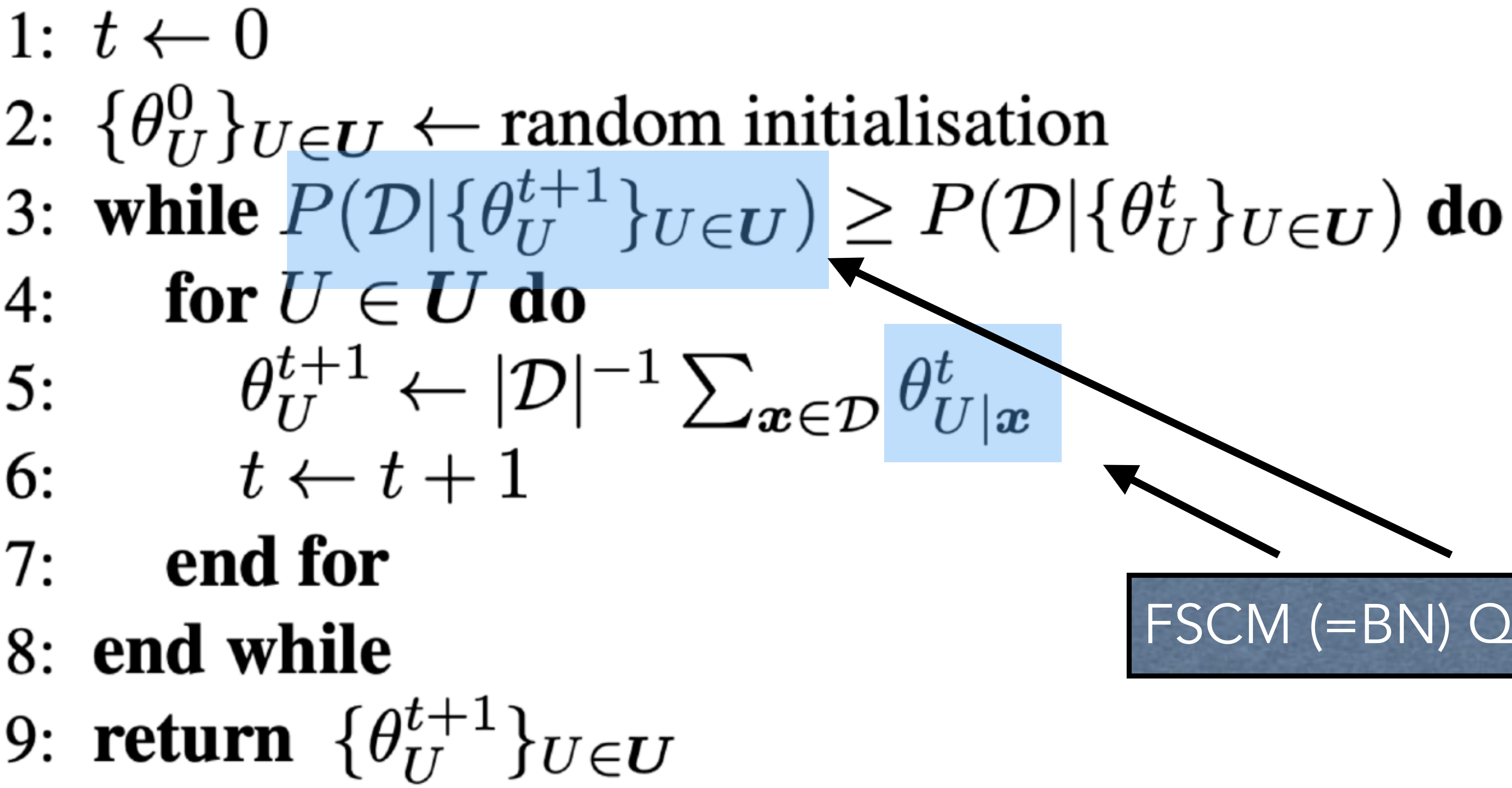
Causal EM (Inferences)



```
$t \leftarrow 0$
$\{\theta_U^0\}_{U\in\boldsymbol{U}} \leftarrow$ random initialisation
while $P(\mathcal{D}|\{\theta_U^{t+1}\}_{U\in\boldsymbol{U}}) \geq P(\mathcal{D}|\{\theta_U^t\}_{U\in\boldsymbol{U}})$ do
    for $U \in \boldsymbol{U}$ do
        $\theta_U^{t+1} \leftarrow |\mathcal{D}|^{-1}\sum_{\boldsymbol{x}\in\mathcal{D}} \theta^t_{U|\boldsymbol{x}}$
        $t \leftarrow t+1$
    end for
end while
return $\{\theta_U^{t+1}\}_{U\in\boldsymbol{U}}$
```

This is a single run, returning exogenous chances to be iterated for different random initialisations

Causal EM (Inferences)



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$t \leftarrow 0$
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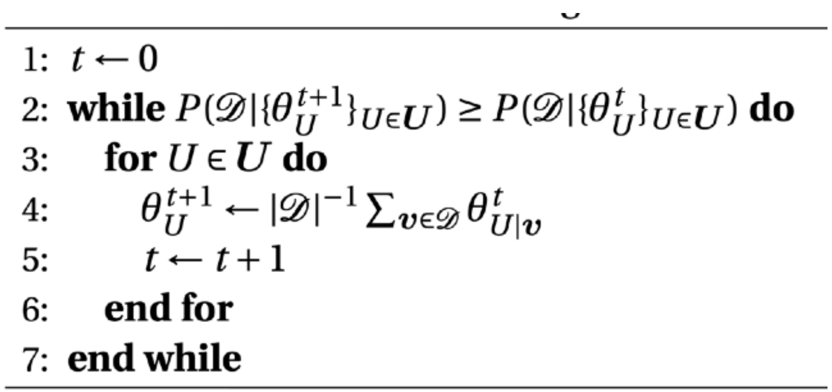
        $t \leftarrow t+1$
    end for
end while
return $\{\theta_U^{t+1}\}_{U \in \boldsymbol{U}}$
```

FSCM (=BN) QUERIES

This is a single run, returning exogenous chances to be iterated for different random initialisations

Speeding up the Causal EM

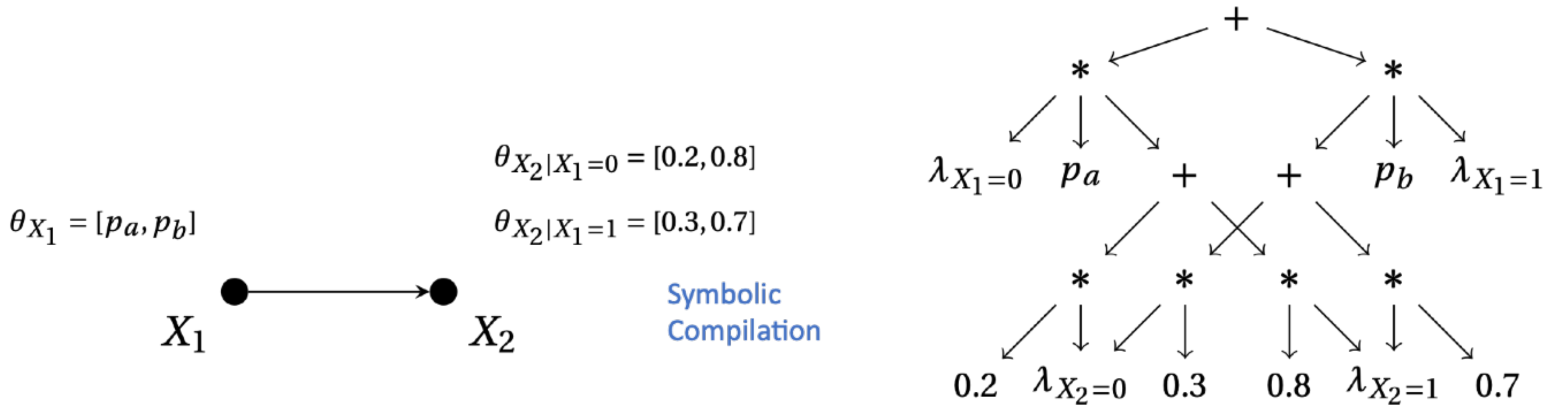
- Parallelisation (on multiple levels)
  - EM initialisations
  - Dataset records
  - (Connected Components)
- Knowledge Compilation?
- EM queries on different models
  - initialisation θ_0
  - iteration t
- Multiple compilations could be expensive, but ...



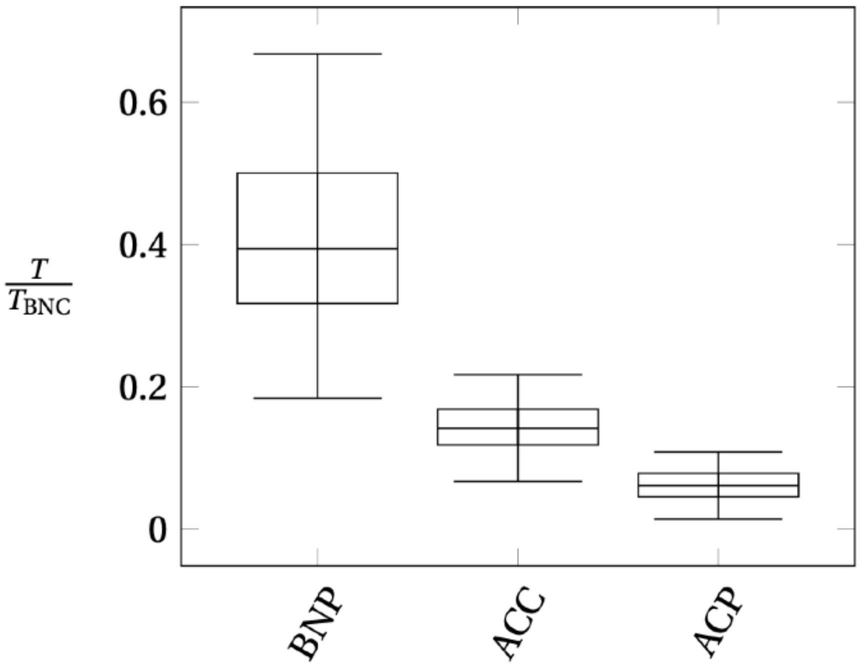
```
$t \leftarrow 0$
while $P(\mathcal{D}|\{\theta_U^{t+1}\}_{U\in\boldsymbol{U}}) \geq P(\mathcal{D}|\{\theta_U^{t}\}_{U\in\boldsymbol{U}})$ do
    for $U \in \boldsymbol{U}$ do
        $\theta_U^{t+1} \leftarrow |\mathcal{D}|^{-1}\sum_{\boldsymbol{v}\in\mathcal{D}}\theta_{U|\boldsymbol{v}}^{t}$
        $t \leftarrow t+1$
    end for
end while
```

Symbolic Knowledge Compilation

- Multiple inferences on different FSCM models
- All FSCMs have a shared structure:
  - Same variables and graph
  - Same equations (endogenous CPTs)
- A "symbolic" (parametrised) compilation
- A single compilation with unique parameters (used as IDs)
- Re-compilation by changing the parameters (linear time wrt pars)



Preliminary Experiments



BNP: Parallelized Variable Eliminations
ACC: Symbolic Knowledge Compilation
ACP: Parallelized Symbolic Knowledge Compilation

Credici
Credal Inference for Causal Inference

+ ACE Compiler

- Symbolic compilation more effective than (component) parallelisation
- ACE exploits the determinism in the structural equations
- Overall, one order of magnitude faster with parallelisation + KC

Conclusions and (a Lot of) Future Work

- Conclusions
  - Concept of parametrised compilation of circuits
  - Knowledge compilation to tractable arithmetic circuits achieves SOTA performance in counterfactual bounding
- Future Work
  - Specialised compilation for SCMs? Canonical equations (FO?), connected components (Decomposed?) and counterfactual graphs (Lifted Inference?)
  - Query-aware methods? (current are query-agnostic)
  - Genuine symbolic inference ("credal" causal EM)
  - Better parallelisation (Julia)