

Logic & Probabilistic Circuits

Representation

Reasoning

Theory

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Objective

- Circuits are an assembly language for tractable logic and probabilistic reasoning
- Even though logic is central to this Simons program, we will couch this tutorial in probability...
 - Most AI and DB interest in tractable logic circuits for the past 15 years has been as a means of doing probabilistic inference
 - Much richer query languages <3
 - We live in the age of probabilistic *generative AI*... :-)
- We will spare you most of the machine learning details, and instead focus on representations, query languages, reasoning algorithms, and connections to theory.

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Questions to be answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
3. *What is the connection to logical circuit languages?* (YooJung)
4. *How do I compile my favorite model into a circuit?* (YooJung)
5. *How are circuit size and tractability related?* (YooJung)
6. *What's the most impressive query we can efficiently compute?* (YooJung)
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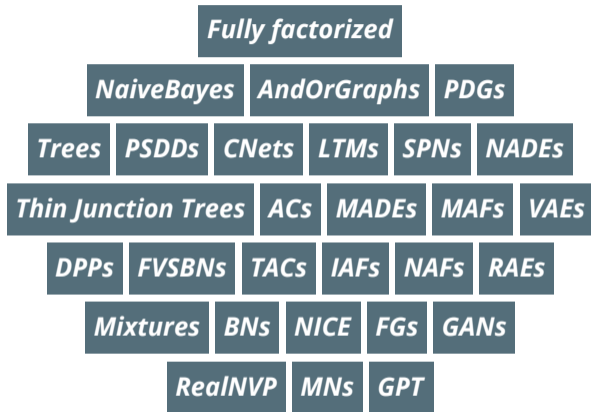
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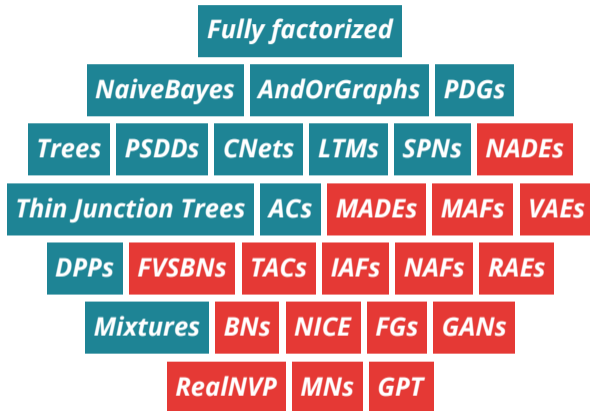
Acknowledgements

This tutorial is based on our (joint) tutorials and slides from

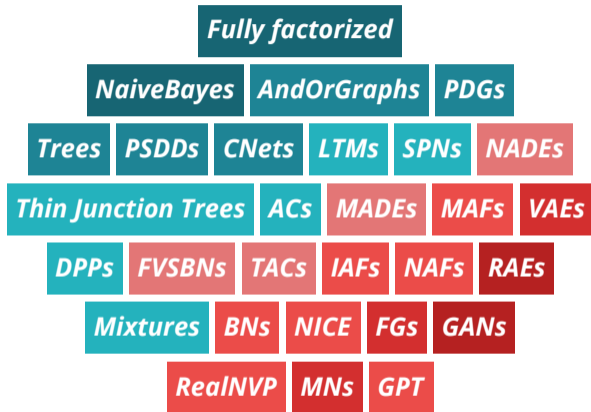
- Antonio Vergari
- Robert Peharz
- Nicola Di Mauro
- Honghua Zhang
- Benjie Wang



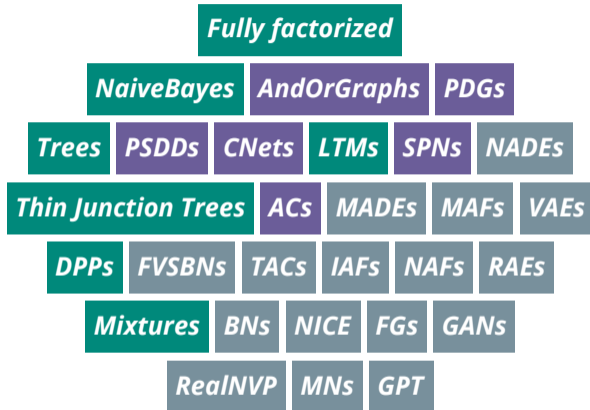
The Alphabet Soup of probabilistic models



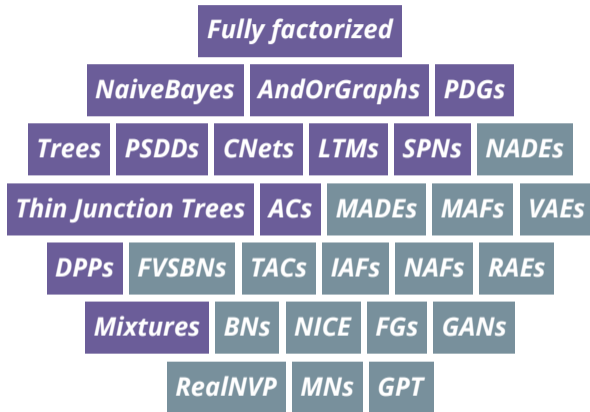
Intractable and ***tractable*** models



tractability is a spectrum



Expressive* models without *compromises



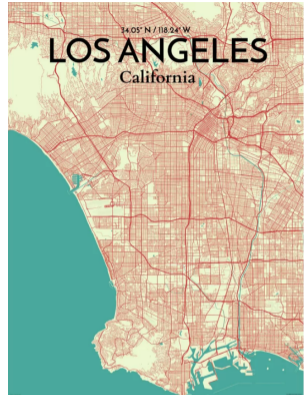
a *unifying framework* for tractable models

Why tractable inference?

or the inherent trade-off of tractability vs. expressiveness

Why probabilistic inference?

q₁: *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*



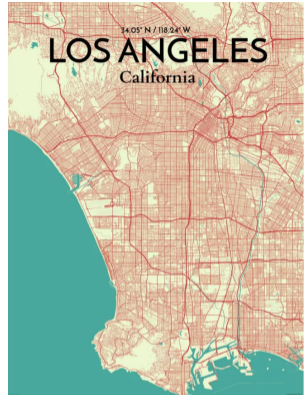
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Why probabilistic inference?

q_1 : *What is the probability that today is a Monday and there is a traffic jam on Westwood Blvd.?*

$\mathbf{X} = \{\text{Day, Time, Jam}_{\text{Str1}}, \text{Jam}_{\text{Str2}}, \dots, \text{Jam}_{\text{StrN}}\}$

$q_1(\mathbf{m}) = p_{\mathbf{m}}(\text{Day} = \text{Mon}, \text{Jam}_{\text{Wwood}} = 1)$



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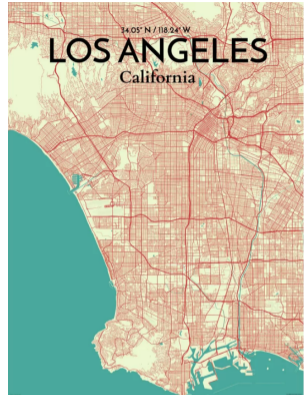
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\Rightarrow *marginals*



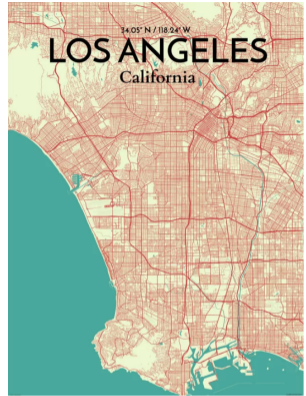
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Why probabilistic inference?

q_2 : Which day is most likely to have a traffic jam on my route to campus?

$\mathbf{X} = \{\text{Day}, \text{Time}, \text{Jam}_{\text{Str}1}, \text{Jam}_{\text{Str}2}, \dots, \text{Jam}_{\text{Str}N}\}$

$q_2(\mathbf{m}) = \operatorname{argmax}_d p_{\mathbf{m}}(\text{Day} = d \wedge \bigvee_{i \in \text{route}} \text{Jam}_{\text{Str}i})$



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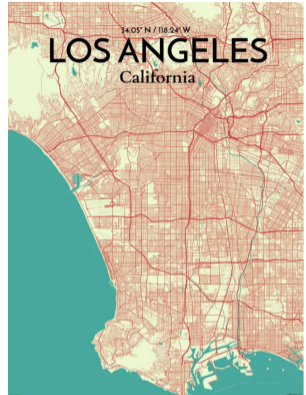
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\Rightarrow *marginals + MAP + logical events*



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Tractable Probabilistic Inference

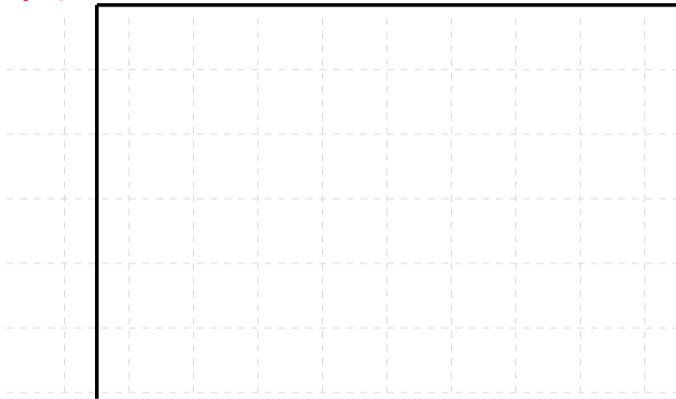
A class of queries \mathcal{Q} is tractable on a family of probabilistic models \mathcal{M} iff for any query $q \in \mathcal{Q}$ and model $m \in \mathcal{M}$ **exactly** computing $q(m)$ runs in time $O(\text{poly}(|m|))$.

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iff for any query $q \in \mathcal{Q}$ and model $m \in \mathcal{M}$
exactly computing $q(m)$ runs in time $O(\text{poly}(|m|))$.

\Rightarrow often poly will in fact be **linear!**

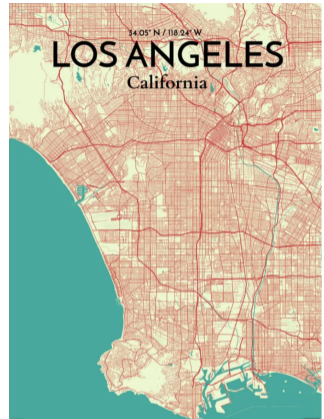
M $Q:$



tractable bands

Complete evidence (EVI)

q₃: *What is the probability that today is a Monday at 12.00 and there is a traffic jam only on Westwood Blvd.?*



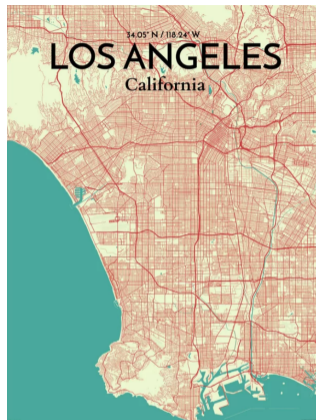
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Complete evidence (EVI)

q_3 : What is the probability that today is a Monday at 12.00 and there is a traffic jam only on Westwood Blvd.?

$\mathbf{X} = \{\text{Day, Time, Jam}_{\text{Wwood}}, \text{Jam}_{\text{Str2}}, \dots, \text{Jam}_{\text{StrN}}\}$

$q_3(\mathbf{m}) = p_{\mathbf{m}}(\mathbf{X} = \{\text{Mon, 12.00, 1, 0}, \dots, 0\})$



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Complete evidence (EVI)

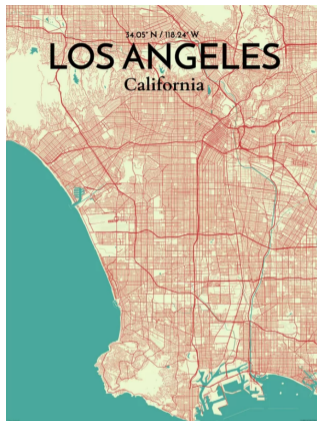
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...fundamental in **maximum likelihood learning**

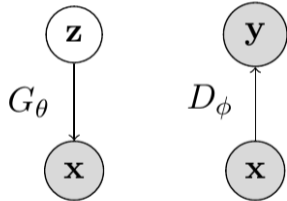
$$\theta_{\mathbf{m}}^{\text{MLE}} = \operatorname{argmax}_{\theta} \prod_{\mathbf{x} \in \mathcal{D}} p_{\mathbf{m}}(\mathbf{x}; \theta)$$



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Generative Adversarial Networks

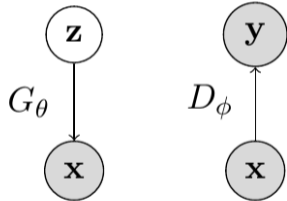
$$\min_{\theta} \max_{\phi} \mathbb{E}_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x})} [\log D_{\phi}(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z})} [\log(1 - D_{\phi}(G_{\theta}(\mathbf{z})))]$$



Generative Adversarial Networks

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- no explicit likelihood!
 - \Rightarrow adversarial training instead of MLE
 - \Rightarrow no tractable ELBO
- good sample quality
 - \Rightarrow but lots of samples needed for MC
- unstable training \Rightarrow mode collapse



M

Q:

EVI

GANs

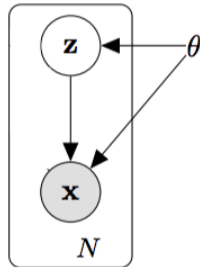


tractable bands

Variational Autoencoders

$$p_{\theta}(\mathbf{x}) = \int p_{\theta}(\mathbf{x} | \mathbf{z})p(\mathbf{z})d\mathbf{z}$$

- an explicit likelihood model!

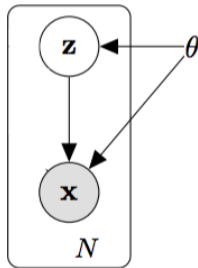


Rezende et al., "Stochastic backprop. and approximate inference in deep generative models", 2014
Kingma and Welling, "Auto-Encoding Variational Bayes", 2014

Variational Autoencoders

$$\log p_{\theta}(\mathbf{x}) \geq \mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z} | \mathbf{x})} [\log p_{\theta}(\mathbf{x} | \mathbf{z})] - \text{KL}(q_{\phi}(\mathbf{z} | \mathbf{x}) || p(\mathbf{z}))$$

- an explicit likelihood model!
- ... but computing $\log p_{\theta}(\mathbf{x})$ is intractable
 - \Rightarrow *an infinite and uncountable mixture*
 - \Rightarrow *no tractable EVI*
- we need to optimize the ELBO...
 - \Rightarrow *which is "tricky"*



\mathcal{M}

\mathcal{Q} :

EVI

GANs

×

VAEs

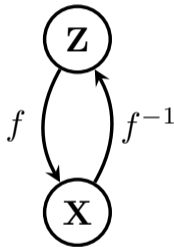
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tractable bands

Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

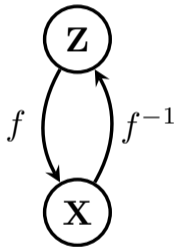
- an explicit likelihood!
 \Rightarrow tractable EVI queries!
- many neural variants
 - RealNVP (*Dinh et al. 2016*),
 MAF (*Papamakarios et al. 2017*)
 - MADE (*Germain et al. 2015*),
 PixelRNN (*Oord et al. 2016*)



Normalizing flows

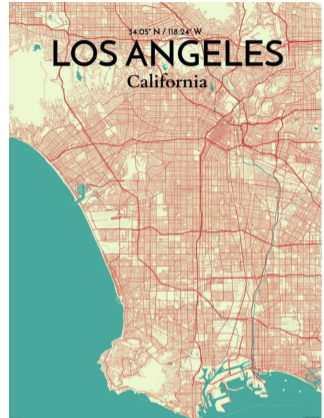
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Marginal queries (MAR)

q_1 : What is the probability that today is a Monday ~~at~~
~~12:00~~ and there is a traffic jam ~~only~~ on Westwood
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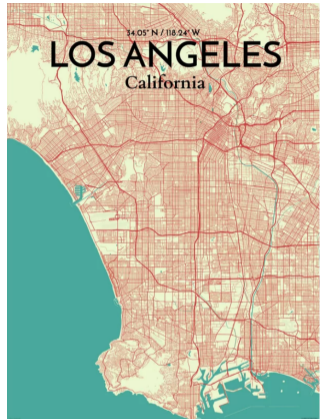


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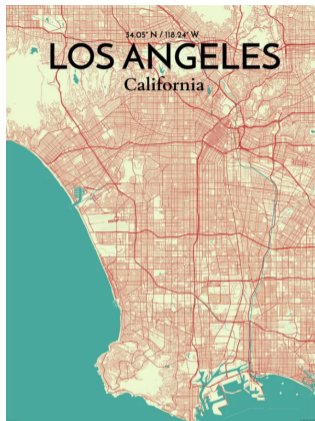
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$$\text{General: } p_{\mathbf{m}}(\mathbf{e}) = \int p_{\mathbf{m}}(\mathbf{e}, \mathbf{H}) d\mathbf{H}$$

$$\text{where } \mathbf{E} \subset \mathbf{X}, \quad \mathbf{H} = \mathbf{X} \setminus \mathbf{E}$$



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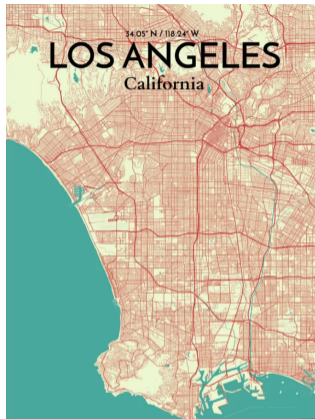
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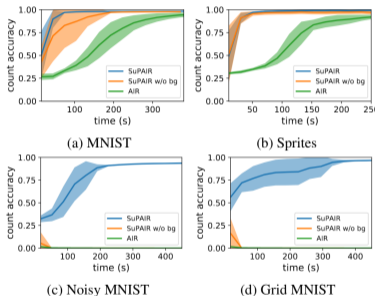
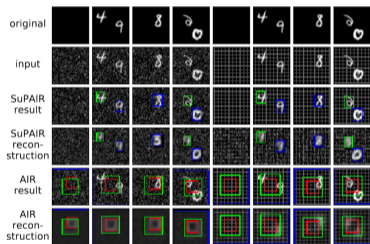
tractable MAR \Rightarrow tractable **conditional queries**
(CON):

$$p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e}) = \frac{p_{\mathbf{m}}(\mathbf{q}, \mathbf{e})}{p_{\mathbf{m}}(\mathbf{e})}$$



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Tractable MAR : scene understanding



Fast and exact marginalization over unseen or “do not care” parts in the scene

Stelzner et al., “Faster Attend-Infer-Repeat with Tractable Probabilistic Models”, 2019

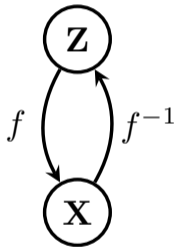
Kossen et al., “Structured Object-Aware Physics Prediction for Video Modeling and Planning”, 2019

Normalizing flows

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(f^{-1}(\mathbf{x})) \left| \det \left(\frac{\delta f^{-1}}{\delta \mathbf{x}} \right) \right|$$

■ an explicit likelihood!

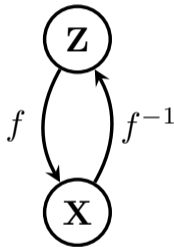
⇒ tractable EVI queries!

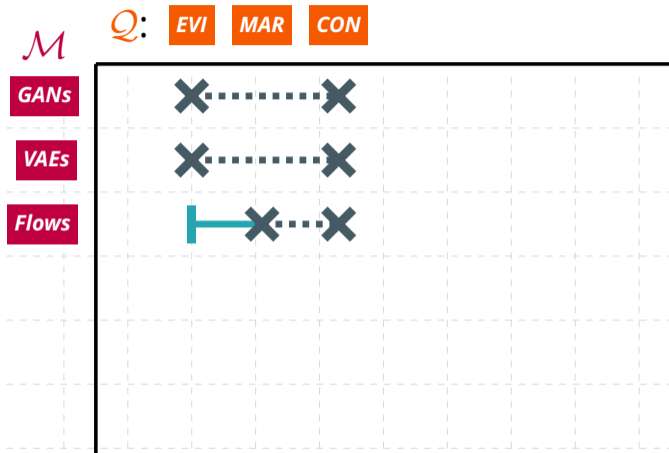


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- an explicit likelihood!
 \Rightarrow tractable EVI queries!
- **MAR is generally intractable:**
we cannot easily integrate over high-dimensional f





tractable bands

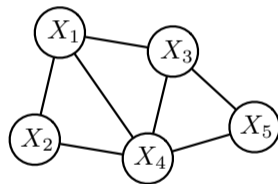
Probabilistic Graphical Models (PGMs)

Declarative semantics: a clean separation of modeling assumptions from inference

Nodes: random variables

Edges: dependencies

+



Inference:

- conditioning (*Darwiche 2001; Sang et al. 2005*)
- elimination (*Zhang et al. 1994; Dechter 1998*)
- message passing (*Yedidia et al. 2001; Dechter et al. 2002; Choi et al. 2010; Sontag et al. 2011*)

Complexity of MAR on PGMs

Exact complexity: Computing MAR and CON is *#P-hard*

⇒ (Cooper 1990; Roth 1996)

Approximation complexity: Computing MAR and CON approximately within a relative error of $2^{n^{1-\epsilon}}$ for any fixed ϵ is *NP-hard*

⇒ (Dagum et al. 1993; Roth 1996)

Treewidth!

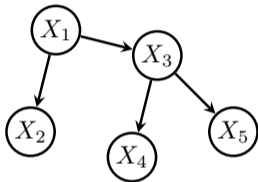
Treewidth:

Informally, how tree-like is the graphical model \mathbf{m} ?

Fixed-parameter tractable: MAR and CON on a graphical model \mathbf{m} with treewidth w take time $O(|\mathbf{X}| \cdot 2^w)$ (Dechter 1998; Koller et al. 2009).

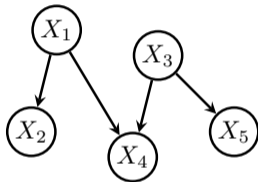
\Rightarrow what about bounding the treewidth by design?

Low-treewidth PGMs



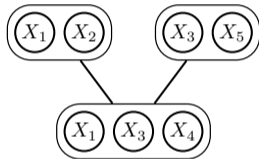
Trees

(Meilă et al. 2000)



Polytrees

(Dasgupta 1999)



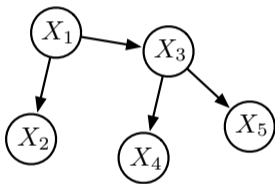
Thin Junction trees

(Bach et al. 2001)

If treewidth is bounded (e.g. ≈ 20), exact MAR and CON inference is possible in practice

Tree distributions

A **tree-structured BN** (Meilă et al. 2000) where each $X_i \in \mathbf{X}$ has *at most* one parent Pa_{x_i} .

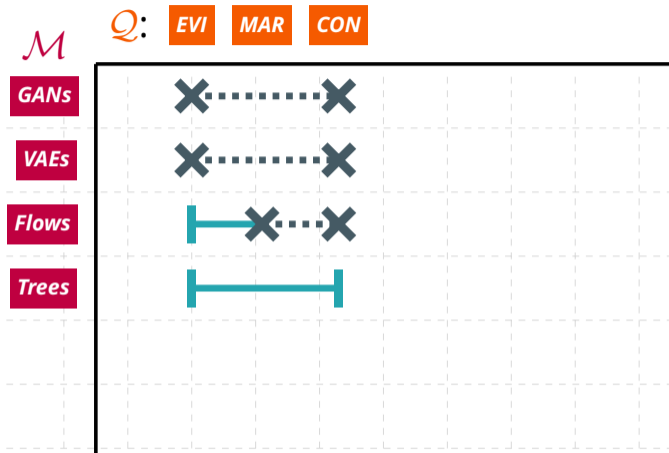


$$p(\mathbf{X}) = \prod_{i=1}^n p(x_i | \text{Pa}_{x_i})$$

Exact querying: EVI, MAR, CON tasks *linear* for trees: $O(|\mathbf{X}|)$

Exact learning from d examples takes $O(|\mathbf{X}|^2 \cdot d)$ with the classical Chow-Liu algorithm¹

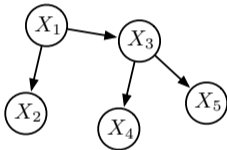
¹Chow et al., "Approximating discrete probability distributions with dependence trees", 1968



tractable bands

What do we lose?

Expressiveness: Ability to represent rich and complex classes of distributions



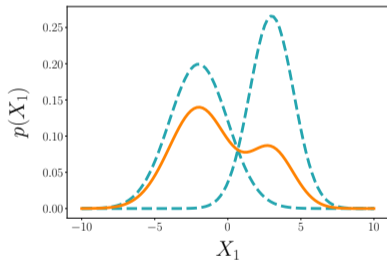
Bounded-treewidth PGMs lose the ability to represent *all possible distributions* ...

Cohen et al., "On the expressive power of deep learning: A tensor analysis", 2016

Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", 2014

Mixtures

Mixtures as a convex combination of k (simpler) probabilistic models

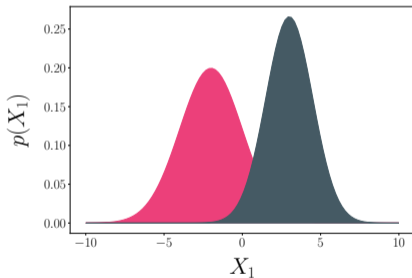


$$p(X) = w_1 \cdot p_1(X) + w_2 \cdot p_2(X)$$

EVI, MAR, CON queries scale linearly in k

Mixtures

Mixtures as a convex combination of k (simpler) probabilistic models



$$p(X) = p(Z = \mathbf{1}) \cdot p_1(X|Z = \mathbf{1}) \\ + p(Z = \mathbf{2}) \cdot p_2(X|Z = \mathbf{2})$$

Mixtures are marginalizing a **categorical latent variable** Z with k values

\Rightarrow *increased expressiveness*

Expressiveness and efficiency

Expressiveness: Ability to represent rich and effective classes of functions

⇒ *mixture of Gaussians can approximate any probability density!*

Cohen et al., "On the expressive power of deep learning: A tensor analysis", 2016
Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", 2014

Expressiveness and efficiency

Expressiveness: Ability to represent rich and effective classes of functions

⇒ *mixture of Gaussians can approximate any probability density!*

Expressive efficiency (aka Succinctness):

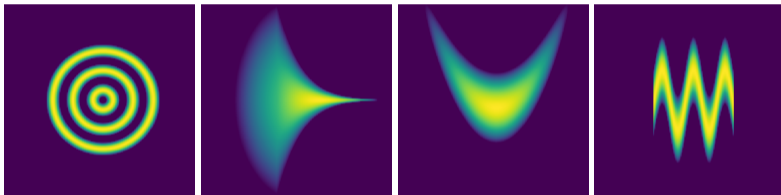
Ability to represent rich and effective classes of functions **compactly**

⇒ *but how many components does a Gaussian mixture need?*

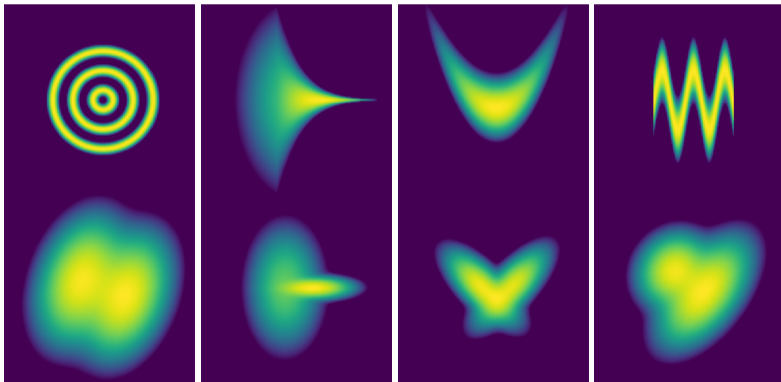
Cohen et al., "On the expressive power of deep learning: A tensor analysis", 2016

Martens and Medabalimi, "On the Expressive Efficiency of Sum Product Networks", 2014

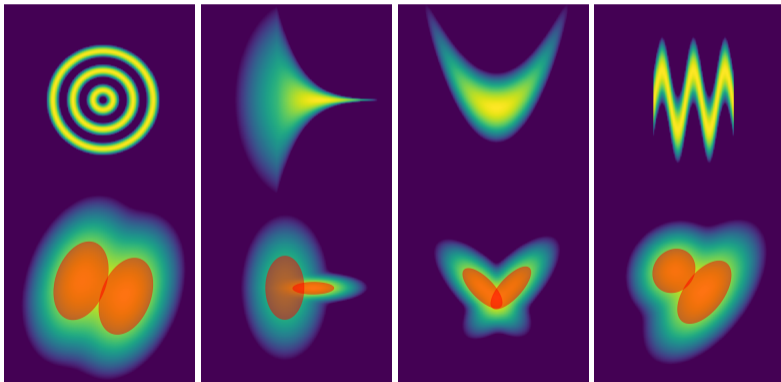
How expressive efficient are mixtures?



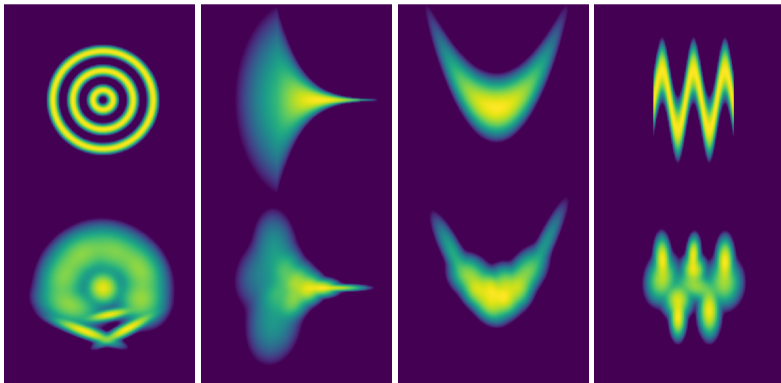
How expressive efficient are mixtures?



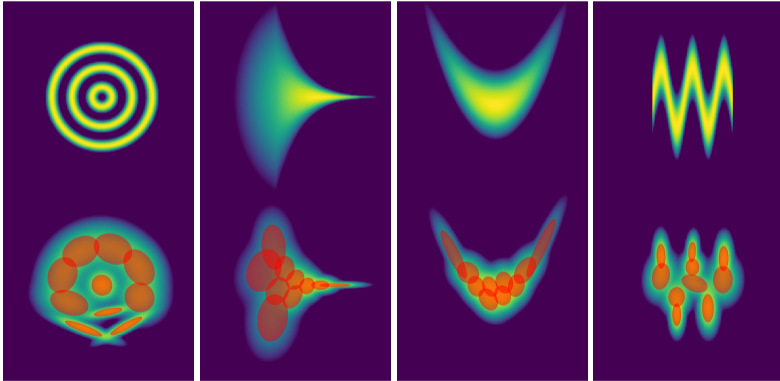
How expressive efficient are mixtures?



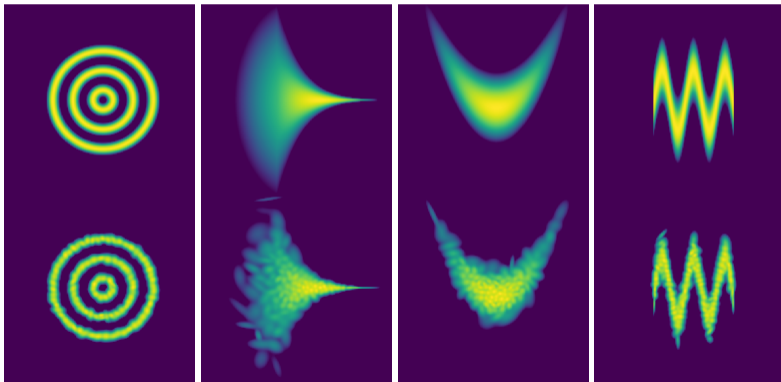
How expressive efficient are mixtures?



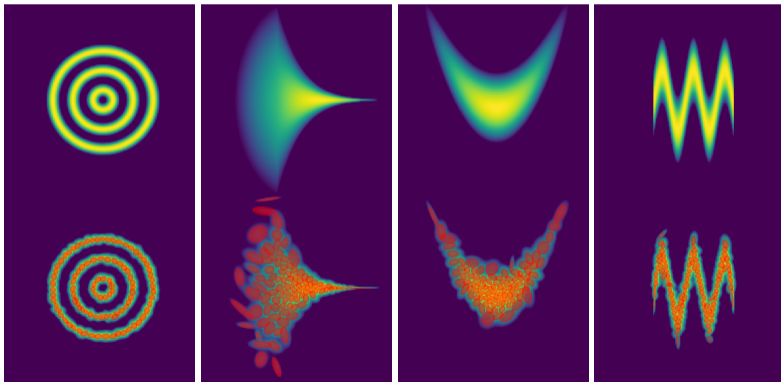
How expressive efficient are mixtures?



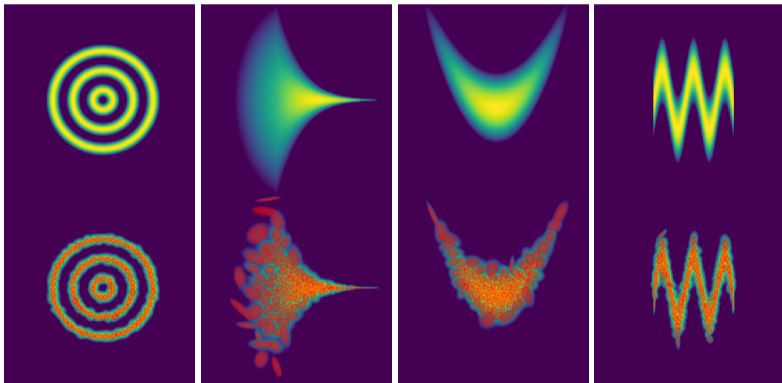
How expressive efficient are mixtures?



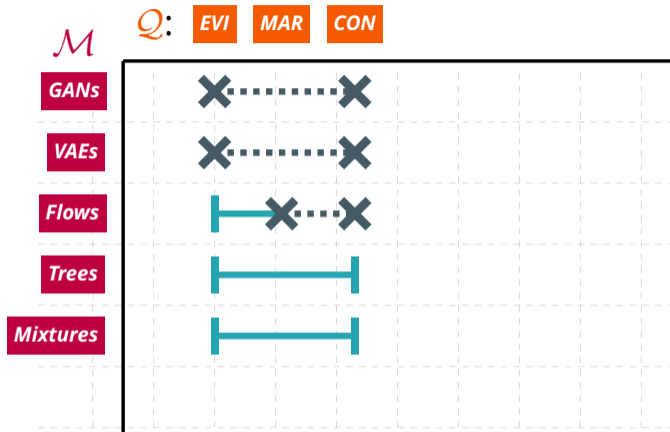
How expressive efficient are mixtures?



How expressive efficient are mixtures?



⇒ *solution: deep mixtures as in deep generative models*

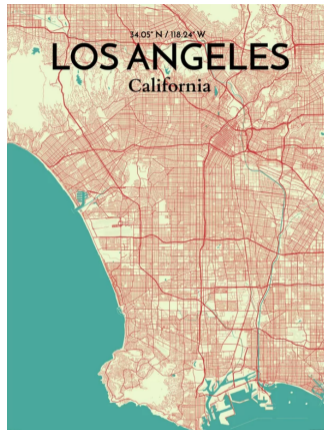


tractable bands

Maximum A Posteriori (MAP)

aka Most Probable Explanation (MPE)

q₅: *Which combination of roads is most likely to be jammed on Monday at 9am?*



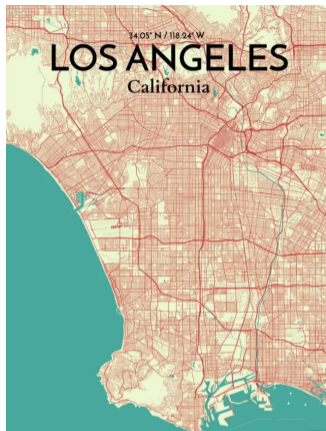
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Maximum A Posteriori (MAP)

aka Most Probable Explanation (MPE)

q₅: Which combination of roads is most likely to be jammed on Monday at 9am?

$$q_5(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \dots \mid \text{Day} = \text{M}, \text{Time} = 9)$$



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Maximum A Posteriori (MAP)

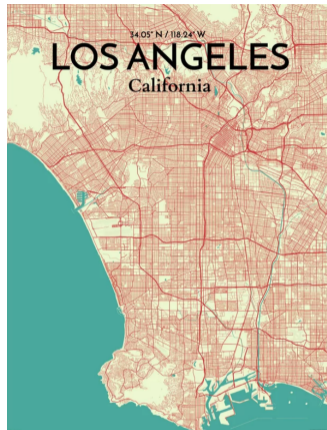
aka Most Probable Explanation (MPE)

q_5 : Which combination of roads is most likely to be jammed on Monday at 9am?

$$q_5(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \dots \mid \text{Day} = \text{M}, \text{Time} = 9)$$

General: $\operatorname{argmax}_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e})$

where $\mathbf{Q} \cup \mathbf{E} = \mathbf{X}$



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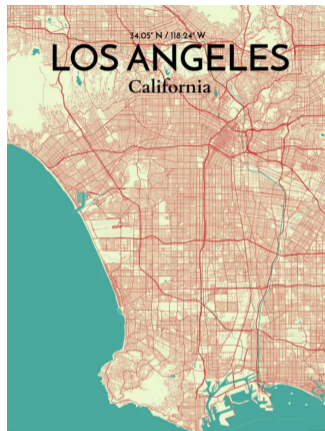
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q₅: Which combination of roads is most likely to be jammed on Monday at 9am?

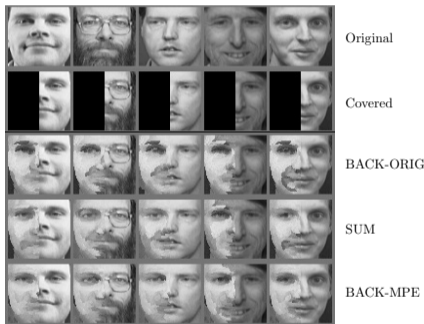
...**intractable** for latent variable models!

$$\begin{aligned}\max_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e}) &= \max_{\mathbf{q}} \sum_{\mathbf{z}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{z} \mid \mathbf{e}) \\ &\neq \sum_{\mathbf{z}} \max_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{z} \mid \mathbf{e})\end{aligned}$$



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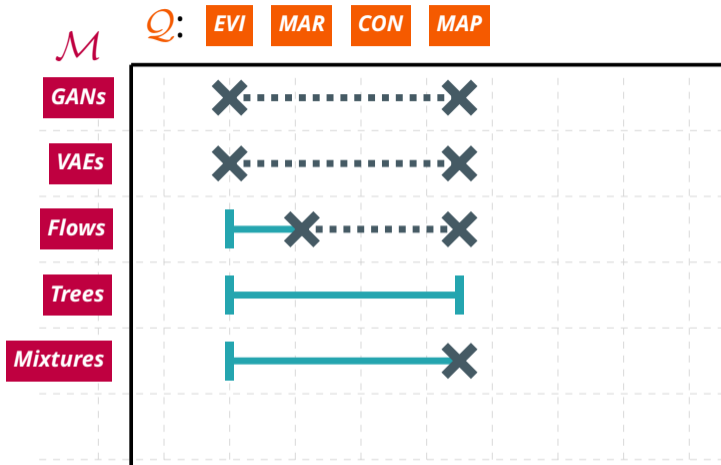
MAP inference : image inpainting



Predicting **arbitrary patches** given a **single** model without the need of retraining.

Poon and Domingos, "Sum-Product Networks: a New Deep Architecture", 2011

Sguerra and Cozman, "Image classification using sum-product networks for autonomous flight of micro aerial vehicles", 2016

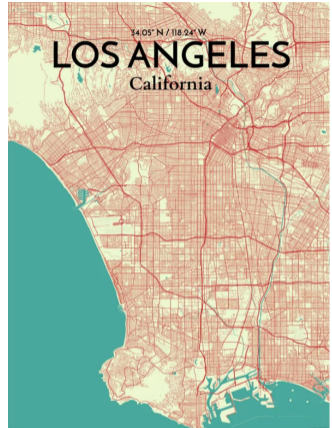


tractable bands

Marginal MAP (MMAP)

aka Bayesian Network MAP

Q₆: Which combination of roads is most likely to be jammed ~~on Monday~~ at 9am?



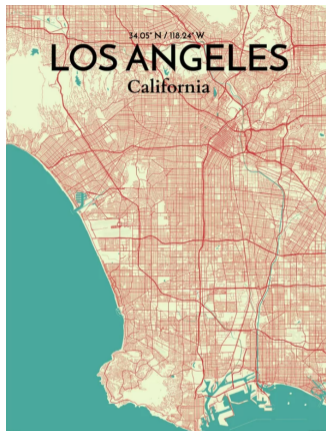
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Marginal MAP (MMAP)

aka Bayesian Network MAP

q₆: Which combination of roads is most likely to be jammed ~~on Monday~~ at 9am?

$$q_6(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \dots \mid \text{Time}=9)$$



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Marginal MAP (MMAP)

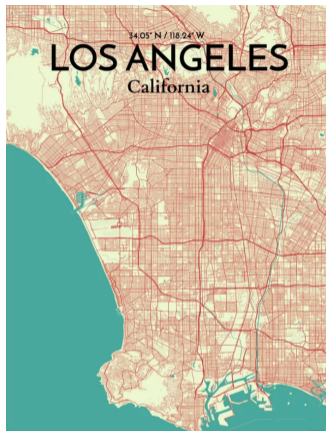
aka Bayesian Network MAP

q_6 : Which combination of roads is most likely to be jammed ~~on Monday~~ at 9am?

$$q_6(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \dots \mid \text{Time}=9)$$

$$\begin{aligned} \text{General: } & \operatorname{argmax}_{\mathbf{q}} p_{\mathbf{m}}(\mathbf{q} \mid \mathbf{e}) \\ & = \operatorname{argmax}_{\mathbf{q}} \sum_{\mathbf{h}} p_{\mathbf{m}}(\mathbf{q}, \mathbf{h} \mid \mathbf{e}) \end{aligned}$$

where $\mathbf{Q} \cup \mathbf{H} \cup \mathbf{E} = \mathbf{X}$



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Marginal MAP (MMAP)

aka Bayesian Network MAP

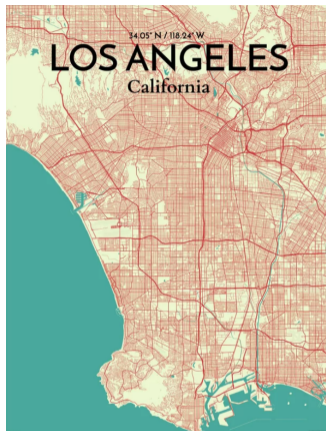
q_6 : Which combination of roads is most likely to be jammed ~~on Monday~~ at 9am?

$$q_6(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}} p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \dots \mid \text{Time}=9)$$

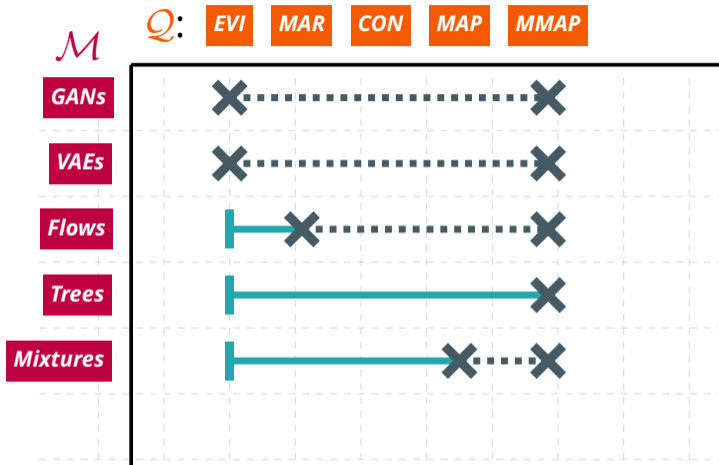
\Rightarrow NP^{PP} -complete (Park et al. 2006)

\Rightarrow NP-hard for trees (de Campos 2011)

\Rightarrow NP-hard even for Naive Bayes (ibid.)



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tractable bands

Advanced queries

q₂: Which day is most likely to have a traffic jam on my route to campus?



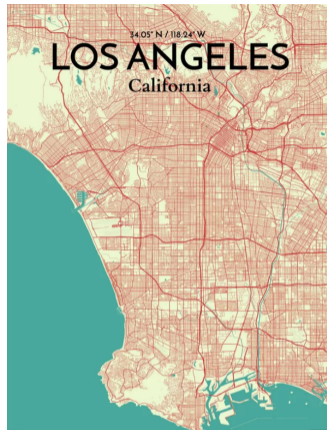
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Advanced queries

q₂: Which day is most likely to have a traffic jam on my route to campus?

$$q_2(\mathbf{m}) = \operatorname{argmax}_d p_{\mathbf{m}}(\text{Day} = d \wedge \bigvee_{i \in \text{route}} \text{Jam}_{\text{Str } i})$$

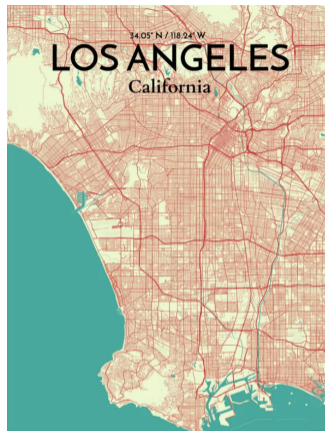
⇒ **marginals + MAP + logical events**



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Advanced queries

- q₂**: Which day is most likely to have a traffic jam on my route to campus?
- q₇**: What is the probability of seeing more traffic jams in Westwood than Hollywood?



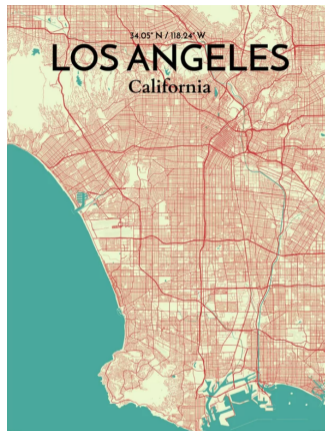
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Advanced queries

q₂: Which day is most likely to have a traffic jam on my route to campus?

q₇: What is the probability of seeing more traffic jams in Westwood than Hollywood?

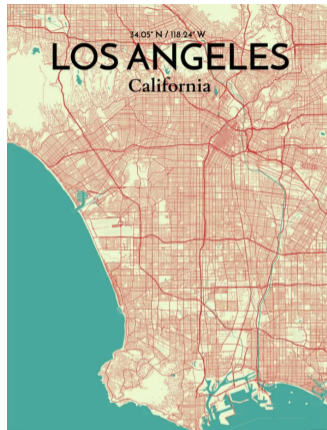
⇒ **counts + group comparison**



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Advanced queries

- q₂**: Which day is most likely to have a traffic jam on my route to campus?
- q₇**: What is the probability of seeing more traffic jams in Westwood than Hollywood?
- q₈**: Is traffic more uncertain on weekdays?

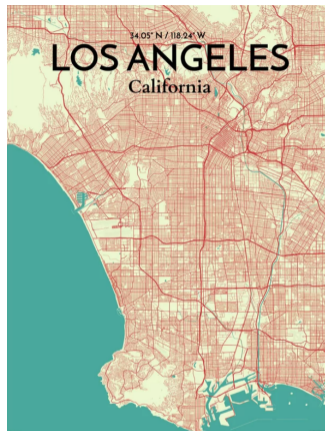


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Advanced queries

- q₂**: Which day is most likely to have a traffic jam on my route to campus?
- q₇**: What is the probability of seeing more traffic jams in Westwood than Hollywood?
- q₈**: Is traffic more uncertain on weekdays?

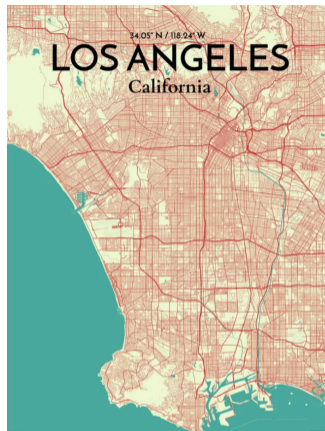
⇒ **information-theoretic queries**



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Advanced queries

- q₂: Which day is most likely to have a traffic jam on my route to campus?
- q₇: What is the probability of seeing more traffic jams in Westwood than Hollywood?
- q₈: Is traffic more uncertain on weekdays?
- q₉: What is the causal effect of doing road works?



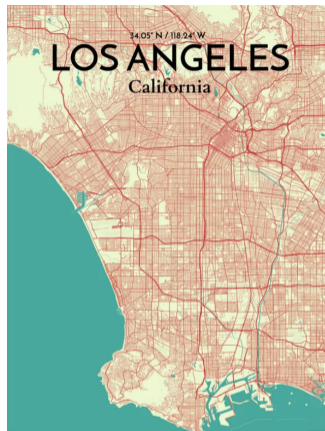
© fineartamerica.com

Advanced queries

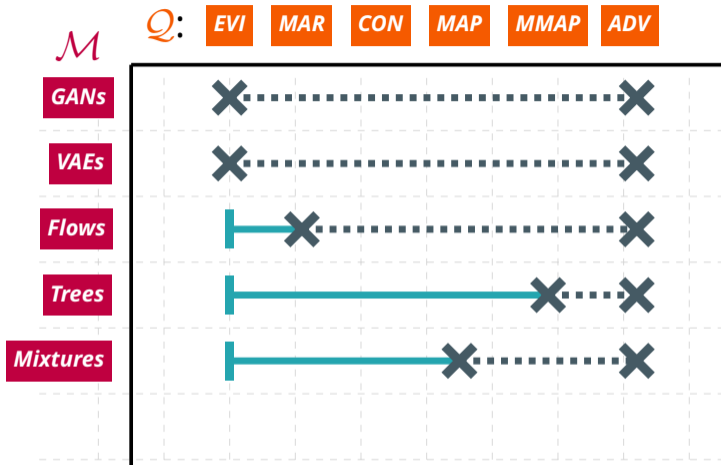
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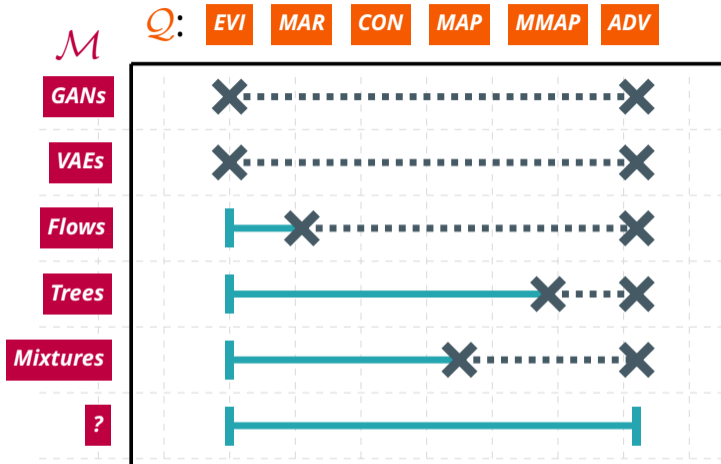
causal backdoor estimation



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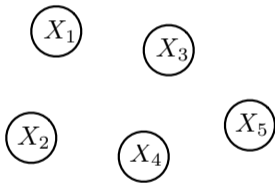
tractable bands



tractable bands

Fully factorized models

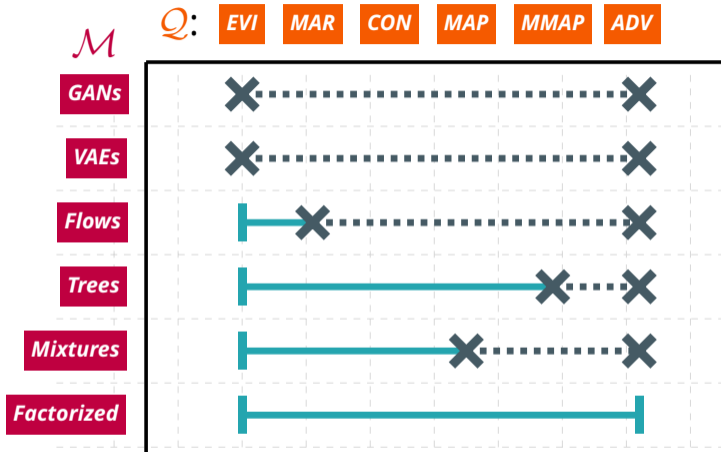
A completely disconnected graph. Example: Product of Bernoullis (PoBs)



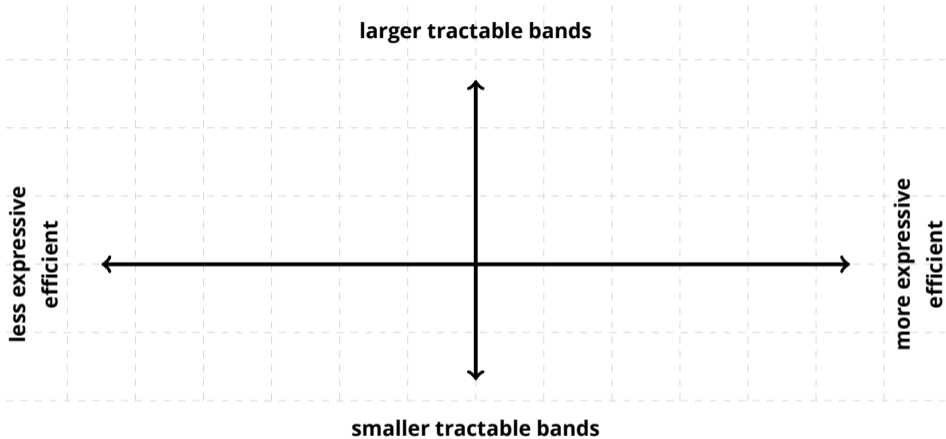
$$p(\mathbf{x}) = \prod_{i=1}^n p(x_i)$$

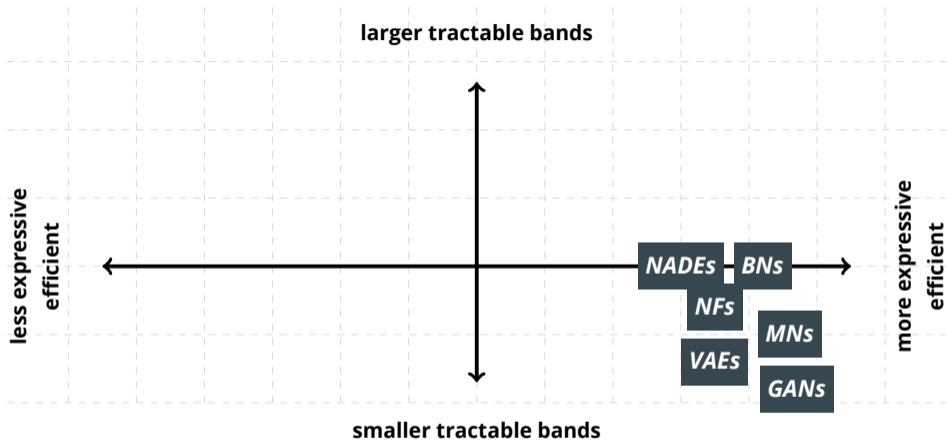
Complete evidence, marginals and MAP, MMAP inference is **linear**!

⇒ *but definitely not expressive...*

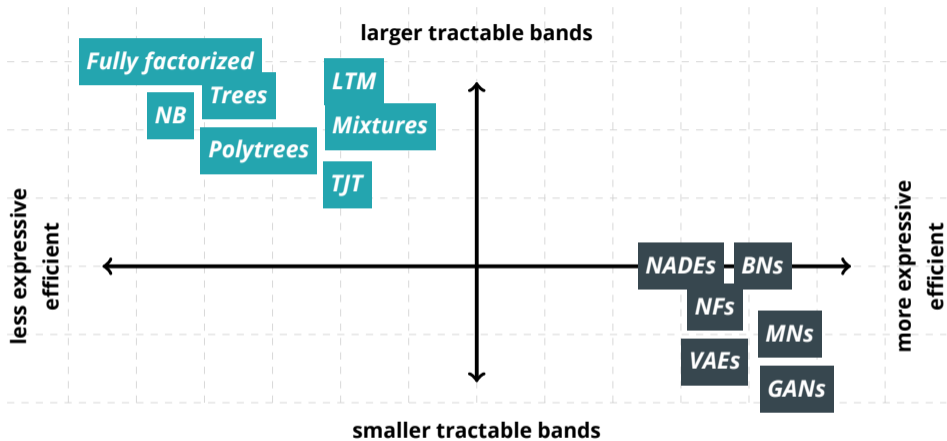


tractable bands

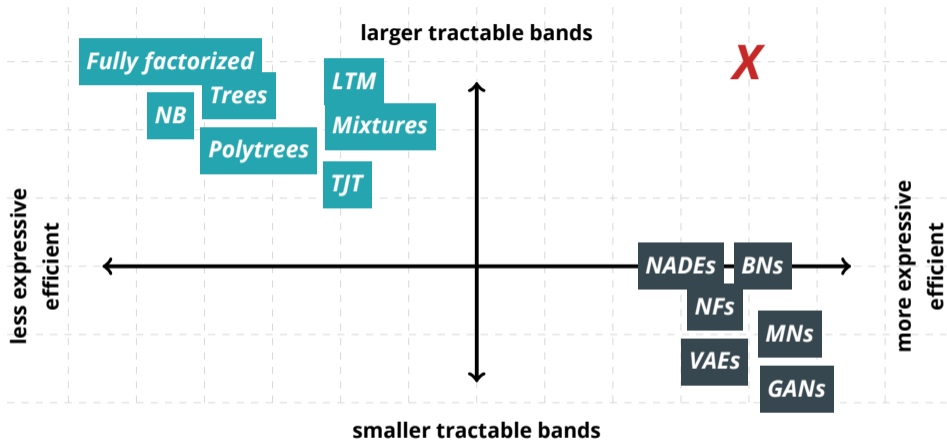




Expressive models are not very tractable...



and tractable ones are not very expressive...



probabilistic circuits are at the "sweet spot"

Questions answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
3. *What is the connection to logical circuit languages?* (YooJung)
4. *How do I compile my favorite model into a circuit?* (YooJung)
5. *How are circuit size and tractability related?* (YooJung)
6. *What's the most impressive query we can efficiently compute?* (YooJung)
7. *Are all tractable distributions probabilistic circuits?* (Guy)
8. *How to learn probabilistic circuits from data?* (Guy)

Questions answered today

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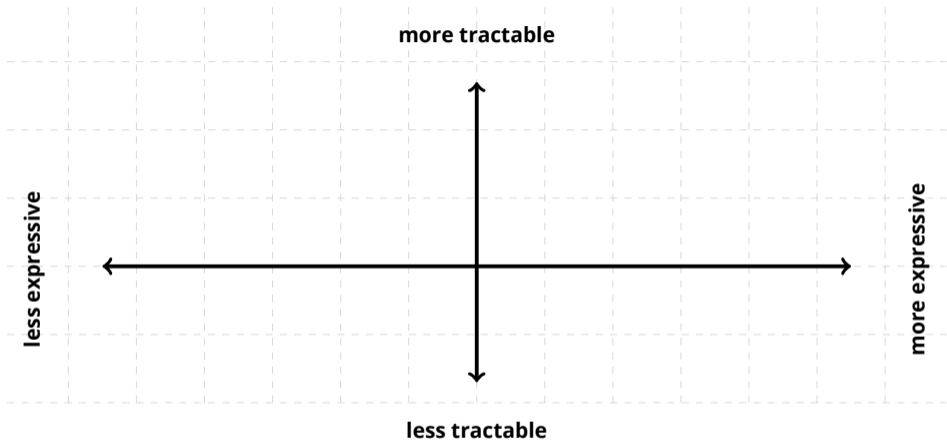
Probabilistic Circuits

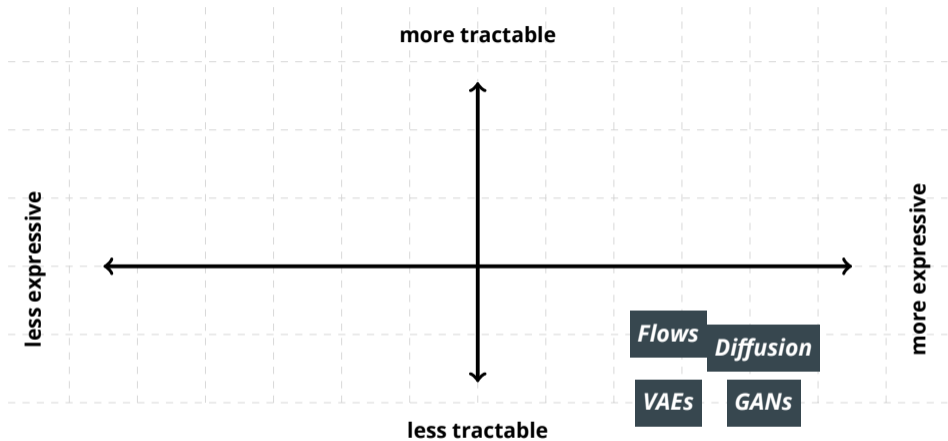
Goal

*Given a reasoning task
can we design
a class of **expressive models**
that is tractable for it?*

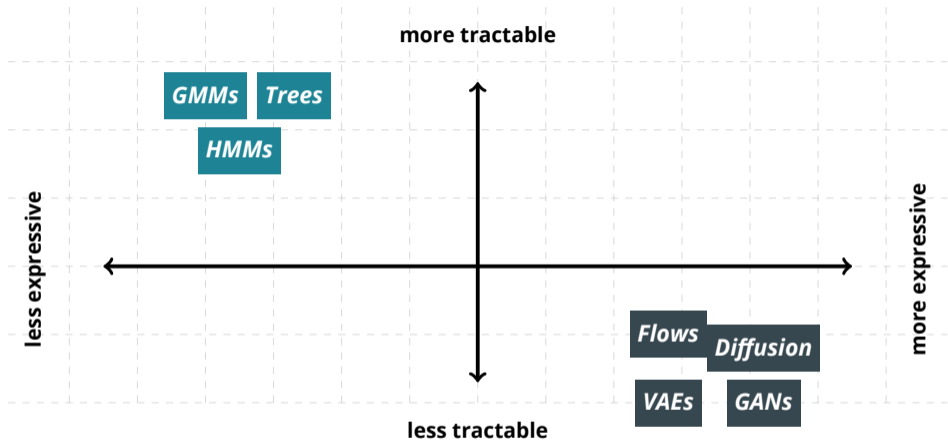
Goal

***Given a reasoning task
can we design
a class of **deep computational graphs**
that is tractable for it?***

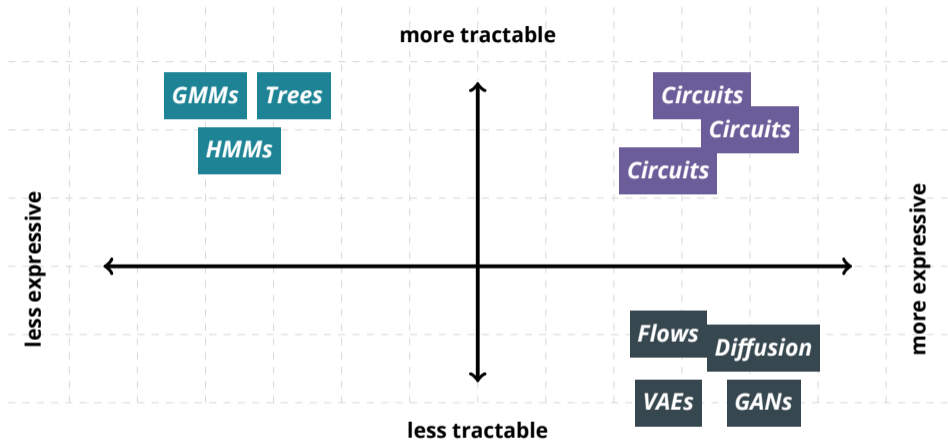




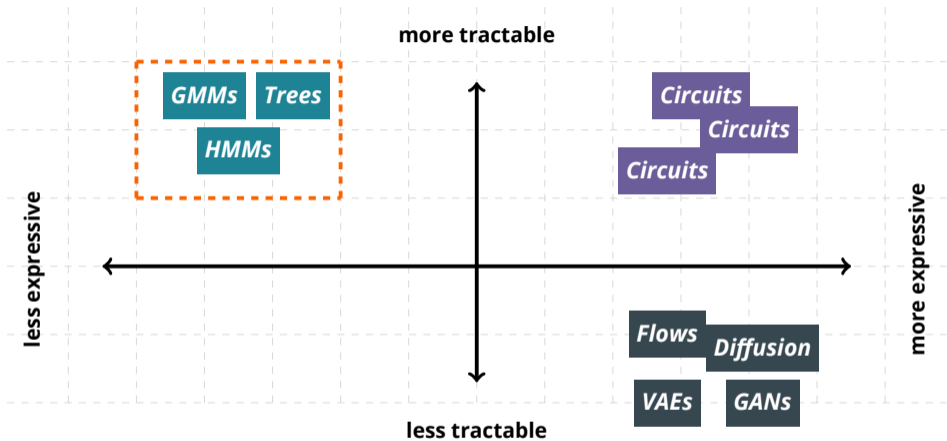
Expressive models are not very tractable...



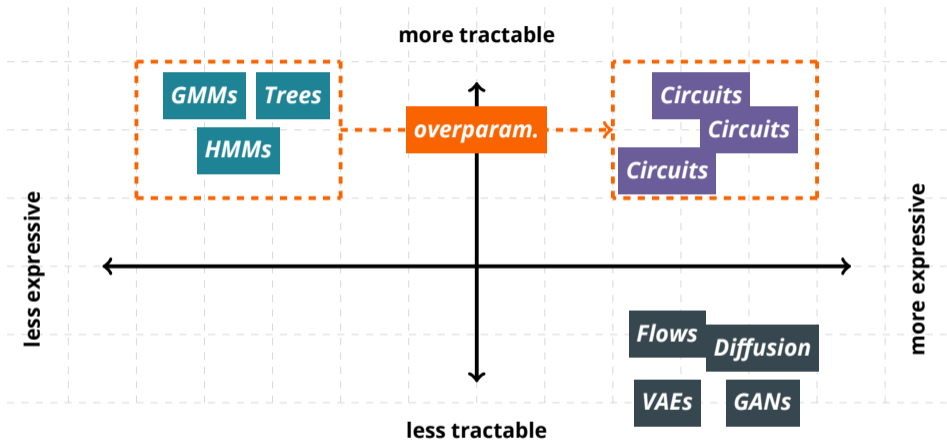
Tractable models are not that expressive...



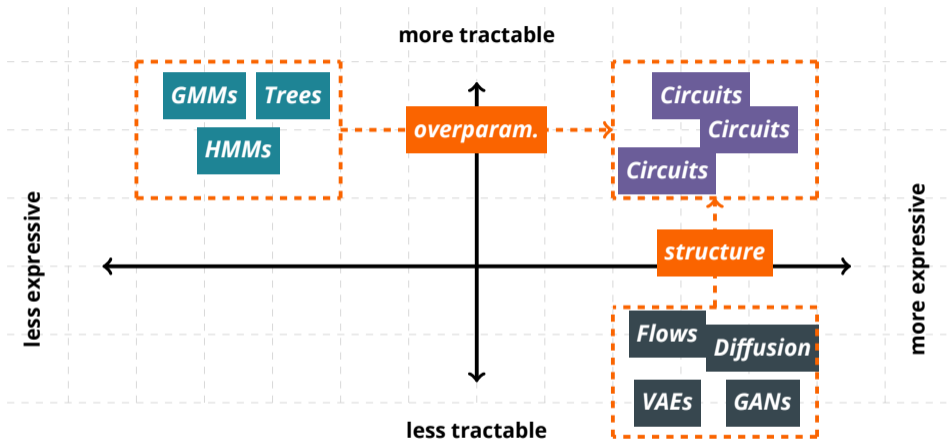
Circuits can be both expressive and tractable!



Start simple...



then make it more expressive!



impose structure!

Input distributions

as computational nodes



Base case: a single node encoding a distribution

\Rightarrow *e.g., Gaussian PDF continuous random variable*

Input distributions

as computational nodes

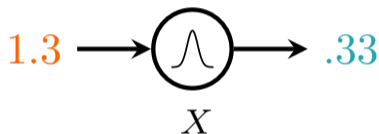


Base case: a single node encoding a distribution

\Rightarrow e.g., indicators for X or $\neg X$ for Boolean random variable

Input distributions

as computational nodes

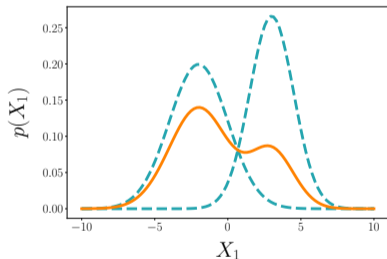


Simple distributions are tractable “black boxes” for:

- EVI: output $p(\mathbf{x})$ (density or mass)
- MAR: output 1 (normalized) or Z (unnormalized)
- MAP: output the mode

Mixture models

as computational graphs

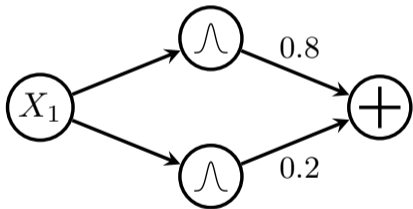


$$p(X) = w_1 \cdot p_1(X_1) + w_2 \cdot p_2(X_1)$$

⇒ *translating inference to data structures...*

Mixture models

as computational graphs

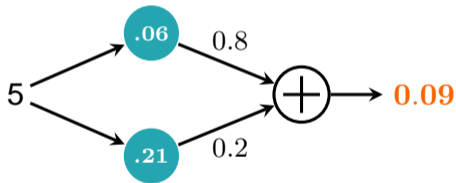


$$p(X_1) = 0.2 \cdot p_1(X_1) + 0.8 \cdot p_2(X_1)$$

⇒ ...e.g., as a weighted sum unit over Gaussian input distributions

Mixture models

as computational graphs

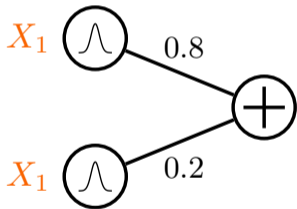


$$p(X = 5) = 0.2 \cdot p_1(X_1 = 5) + 0.8 \cdot p_2(X_1 = 5)$$

\Rightarrow inference = feedforward evaluation

Mixture models

as computational graphs



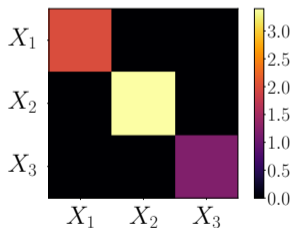
A simplified notation:

- \Rightarrow **scopes** attached to inputs
- \Rightarrow edge directions omitted

Factorizations

as computational graphs

$$p(X_1, X_2, X_3) = p(X_1) \cdot p(X_2) \cdot p(X_3)$$

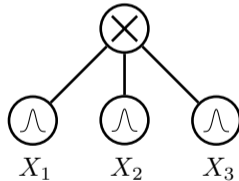
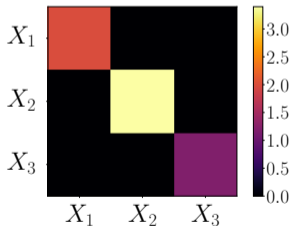


\Rightarrow e.g. modeling a multivariate Gaussian with diagonal covariance matrix...

Factorizations

as computational graphs

$$p(X_1, X_2, X_3) = p(X_1) \cdot p(X_2) \cdot p(X_3)$$

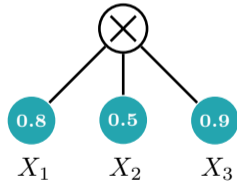
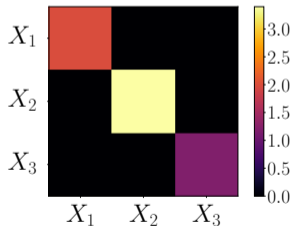


⇒ ...with a product node over some univariate Gaussian distribution

Factorizations

as computational graphs

$$p(x_1, x_2, x_3) = p(x_1) \cdot p(x_2) \cdot p(x_3)$$

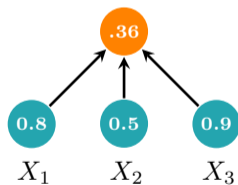
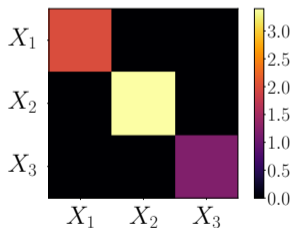


⇒ *feedforward evaluation*

Factorizations

as computational graphs

$$p(x_1, x_2, x_3) = p(x_1) \cdot p(x_2) \cdot p(x_3)$$



⇒ *feedforward evaluation*

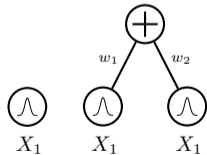
A grammar for tractable models

Recursive semantics of probabilistic circuits



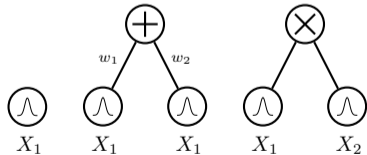
A grammar for tractable models

Recursive semantics of probabilistic circuits



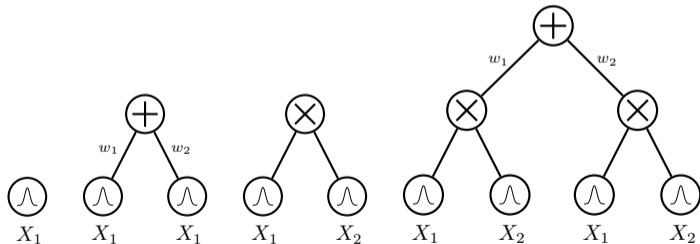
A grammar for tractable models

Recursive semantics of probabilistic circuits



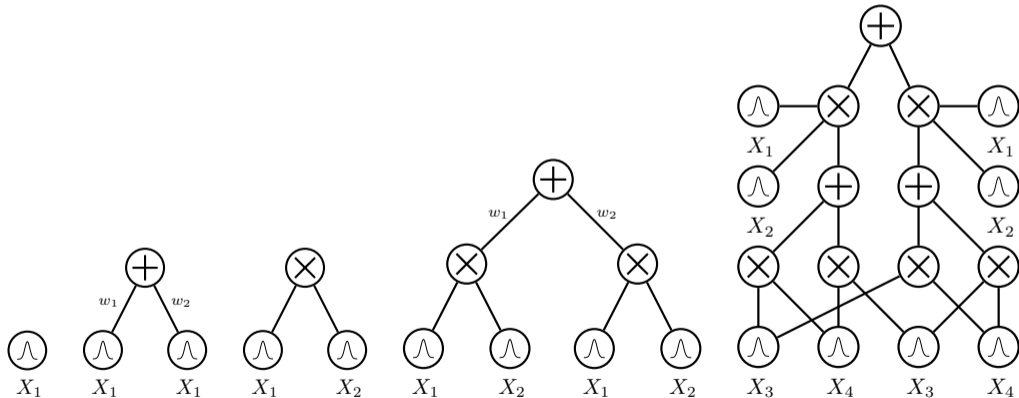
A grammar for tractable models

Recursive semantics of probabilistic circuits



A grammar for tractable models

Recursive semantics of probabilistic circuits



Building PCs in Python with SPFlow

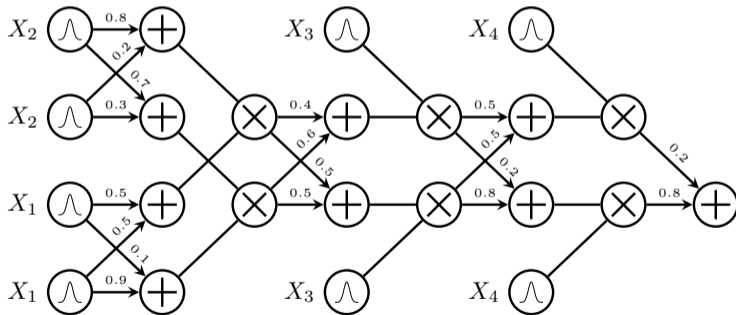


```
import spn.structure.leaves.parametric.Parametric as param
from param import Categorical, Gaussian
```

```
PC = 0.4 * (Categorical(p=[0.2, 0.8], scope=0) *
            (0.3 * (Gaussian(mean=1.0, stdev=1.0, scope=1) *
                    Categorical(p=[0.4, 0.6], scope=2))
            + 0.7 * (Gaussian(mean=-1.0, stdev=1.0, scope=1) *
                    Categorical(p=[0.6, 0.4], scope=2)))) \
+ 0.6 * (Categorical(p=[0.2, 0.8], scope=0) *
         Gaussian(mean=0.0, stdev=0.1, scope=1) *
         Categorical(p=[0.4, 0.6], scope=2))
```

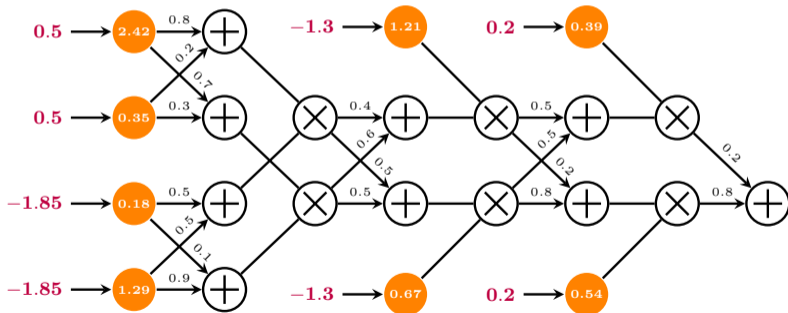
EVI queries = ***feedforward*** evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



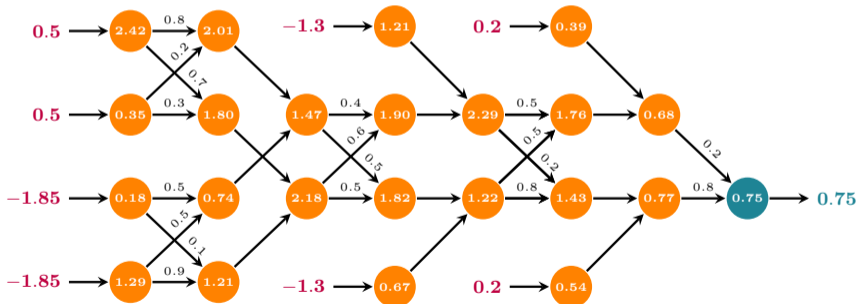
EVI queries = **feedforward** evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$

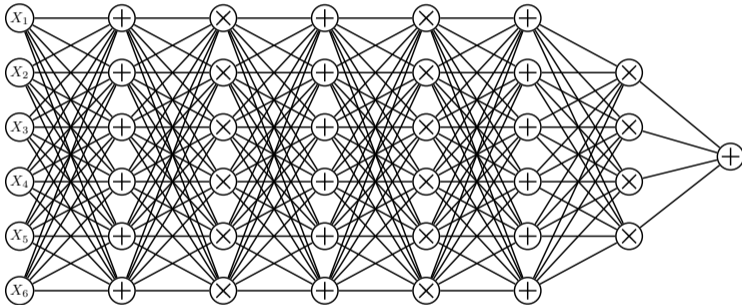


EVI queries = *feedforward* evaluation

$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2) = 0.75$$

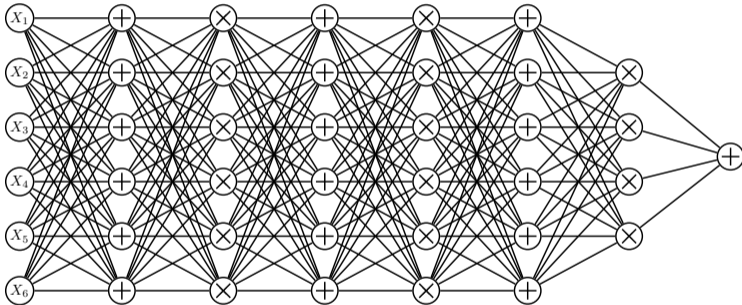


Just sum, products and distributions?



just arbitrarily compose them like a neural network!

Just sum, products and distributions?



~~just arbitrarily compose them like a neural network!~~



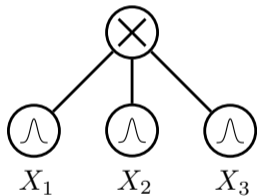
structural properties needed for tractability

***Which structural constraints
ensure tractability?***

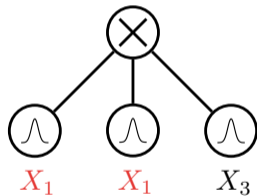
Decomposability

A product node is decomposable if its children depend on disjoint sets of variables

\Rightarrow just like in factorization!



decomposable circuit



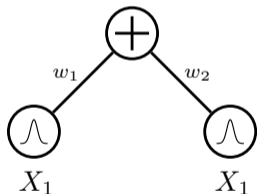
non-decomposable circuit

Smoothness

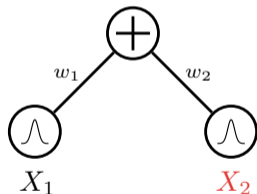
aka completeness

A sum node is smooth if its children depend of the same variable sets

⇒ otherwise not accounting for some variables



smooth circuit



non-smooth circuit

⇒ smoothness can be easily enforced (Shih et al. 2019)

Smoothness + **decomposability** = **tractable MAR**

Computing arbitrary integrations (or summations)

\Rightarrow *linear in circuit size!*

E.g., suppose we want to compute Z
(the distribution's normalizing constant):

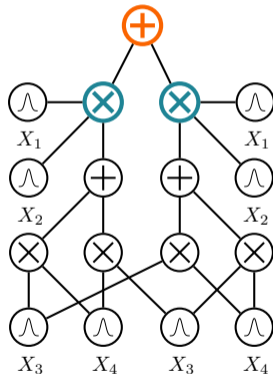
$$\int p(\mathbf{x}) d\mathbf{x}$$

Smoothness + **decomposability** = **tractable MAR**

If $p(\mathbf{x}) = \sum_i w_i p_i(\mathbf{x})$, (**smoothness**):

$$\int p(\mathbf{x}) d\mathbf{x} = \int \sum_i w_i p_i(\mathbf{x}) d\mathbf{x} = \sum_i w_i \int p_i(\mathbf{x}) d\mathbf{x}$$

\Rightarrow integrals are “pushed down” to children

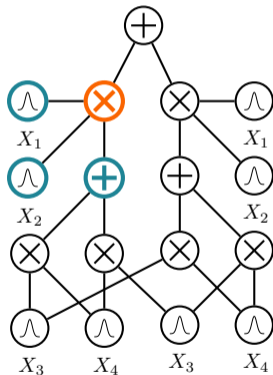


Smoothness + **decomposability** = **tractable MAR**

If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (**decomposability**):

$$\begin{aligned} & \int \int \int p(\mathbf{x}, \mathbf{y}, \mathbf{z}) dx dy dz = \\ &= \int \int \int p(\mathbf{x})p(\mathbf{y})p(\mathbf{z}) dx dy dz = \\ &= \int p(\mathbf{x}) dx \int p(\mathbf{y}) dy \int p(\mathbf{z}) dz \end{aligned}$$

\Rightarrow integrals decompose into easier ones



Smoothness + **decomposability** = **tractable MAR**

Forward pass evaluation for MAR

\Rightarrow linear in circuit size!

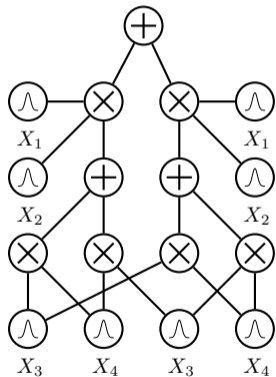
E.g. to compute $p(x_2, x_4)$:

leaves over X_1 and X_3 output $Z_i = \int p(x_i) dx_i$

\Rightarrow for normalized leaf distributions: 1.0

leaves over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)



Smoothness + **decomposability** = **tractable MAR**

Forward pass evaluation for MAR

\Rightarrow linear in circuit size!

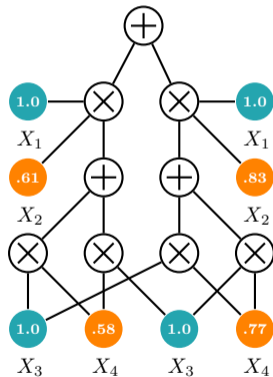
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feedforward evaluation (bottom-up)



Smoothness + **decomposability** = **tractable MAR**

Forward pass evaluation for MAR

\Rightarrow linear in circuit size!

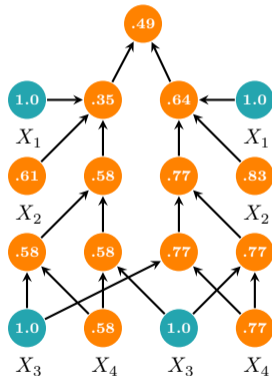
E.g. to compute $p(x_2, x_4)$:

leaves over X_1 and X_3 output $Z_i = \int p(x_i) dx_i$

\Rightarrow for normalized leaf distributions: **1.0**

leaves over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)

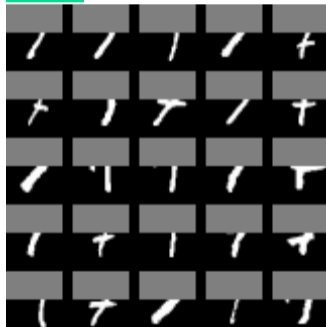


Tractable MAR

EVI 10,958.72 nats



MAR 5,387.55 nats

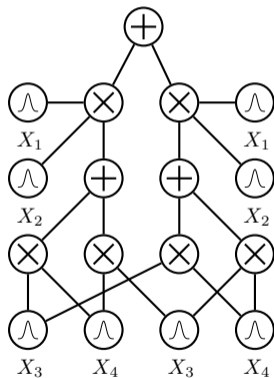


Smoothness + **decomposability** = **tractable CON**

Analogously, for arbitrary conditional queries:

$$p(\mathbf{q} \mid \mathbf{e}) = \frac{p(\mathbf{q}, \mathbf{e})}{p(\mathbf{e})}$$

1. evaluate $p(\mathbf{q}, \mathbf{e}) \Rightarrow$ *one feedforward pass*
2. evaluate $p(\mathbf{e}) \Rightarrow$ *another feedforward pass*
 \Rightarrow *...still linear in circuit size!*

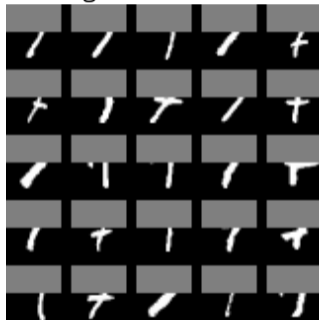


Tractable CON

Original



Missing



Conditional sample



Generative models are still hard to control

more reasoning!

Generate image





Generate a sentence using "frisbee", "caught" and "dog", following the given order.



Generate a sentence using "frisbee", "caught" and "dog", following the given order.



After a perfect throw, the frisbee glided through the air, and the dog, with incredible agility, caught it mid-flight.

ChatGPT



Generate a sentence using "frisbee", "caught" and "dog", following the given order.



After a perfect throw, the frisbee glided through the air, and the dog, with incredible agility, caught it mid-flight.

ChatGPT



That's not correct. Generate a sentence using "frisbee", "caught" and "dog". The keywords should appear in the order as specified.



Here's the correct sentence: The dog caught the frisbee in mid-air, showing off its amazing catching skills.

ChatGPT



Generate a sentence using "frisbee", "caught" and "dog", following the given order.



After a perfect throw, the frisbee glided through the air, and the dog, with incredible agility, caught it mid-flight.

ChatGPT



That's not correct. Generate a sentence using "frisbee", "caught" and "dog". The keywords should appear in the order as specified.



Here's the correct sentence: The dog caught the frisbee in mid-air, showing off its amazing catching skills.

ChatGPT



A frisbee is caught by a dog.

A pair of frisbee players are caught in a dog fight.

GeLaTo

What do we have?

Prefix: “The weather is”

Constraint α : text contains “winter”

Model only does $p(\text{next-token}|\text{prefix}) =$

cold	0.05
warm	0.10

What do we need?

Prefix: “The weather is”

Constraint α : text contains “winter”

Generate from $p(\text{next-token}|\text{prefix}, \alpha) =$

cold	0.50
warm	0.01

$$\propto \sum_{\text{text}} p(\text{next-token}, \text{text}, \text{prefix}, \alpha)$$

Marginalization!

Computing $p(\alpha \mid x_{1:t+1})$

For α in conjunctive normal form (CNF):

$$(w_{1,1} \vee \dots \vee w_{1,d_1}) \wedge \dots \wedge (w_{m,1} \vee \dots \vee w_{m,d_m})$$

where each w_{ij} is a keyword (i.e. a string of tokens),
representing the constraint that w_{ij} appears in the generated text.

e.g., $\alpha = (\text{"swims"} \vee \text{"like swimming"}) \wedge (\text{"lake"} \vee \text{"pool"})$

Computing $p(\alpha \mid x_{1:t+1})$

For α in conjunctive normal form (CNF):

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e.g., $\alpha = (\text{"swims"} \vee \text{"like swimming"}) \wedge (\text{"lake"} \vee \text{"pool"})$

Efficient algorithm:

For m clauses and sequence length n , time-complexity for generation is $O(2^{|m|}n)$
when p is a *hidden Markov model* (see general probabilistic circuit case later).

Trick: dynamic programming with clever preprocessing and local belief updates

CommonGen: a Challenging Benchmark

Given 3-5 concepts (keywords), our goal is to generate a sentence using all keywords, which can appear in any order and any form of inflections. e.g.,

Input: snow drive car

Reference 1: A car drives down a snow covered road.

Reference 2: Two cars drove through the snow.

$$(w_{1,1} \vee \dots \vee w_{1,d_1}) \wedge \dots \wedge (w_{m,1} \vee \dots \vee w_{m,d_m})$$

Each clause represents the inflections for one keyword.

GeLaTo Overview

Lexical Constraint α : sentence contains keyword "winter"

Constrained Generation: $\Pr(x_{t+1} | \alpha, x_{1:t} = \text{"the weather is"})$

✗ intractable

✓ efficient

Pre-trained
Language Model

Tractable
Probabilistic Model

Minimize KL-divergence

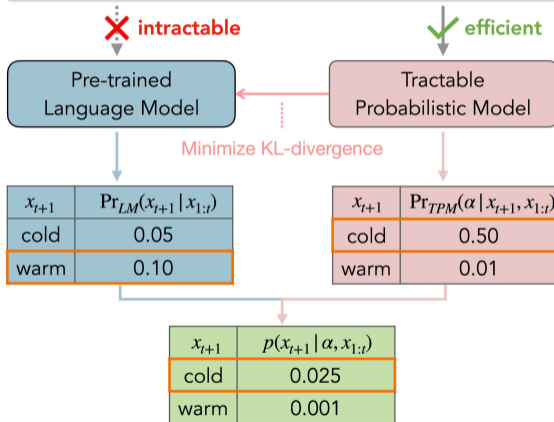
x_{t+1}	$\Pr_{LM}(x_{t+1} x_{1:t})$
cold	0.05
warm	0.10

x_{t+1}	$\Pr_{TPM}(\alpha x_{t+1}, x_{1:t})$
cold	0.50
warm	0.01

GeLaTo Overview

Lexical Constraint α : sentence contains keyword "winter"

Constrained Generation: $\Pr(x_{t+1} | \alpha, x_{1:t} = \text{"the weather is"})$



Step 2: Control p_{gpt} via p_{hmm}

Unsupervised

Language model is not
fine-tuned/prompted to satisfy constraints

By Bayes rule:

$$p_{gpt}(x_{t+1} | x_{1:t}, \alpha) \propto p_{gpt}(\alpha | x_{1:t+1}) \cdot p_{gpt}(x_{t+1} | x_{1:t})$$

Assume $p_{hmm}(\alpha | x_{1:t+1}) \approx p_{gpt}(\alpha | x_{1:t+1})$, we
generate from:

$$p(x_{t+1} | x_{1:t}, \alpha) \propto p_{hmm}(\alpha | x_{1:t+1}) \cdot p_{gpt}(x_{t+1} | x_{1:t})$$

Method	Generation Quality								Constraint Satisfaction			
	ROUGE-L		BLEU-4		CIDEr		SPICE		Coverage		Success Rate	
	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>
<i>Unsupervised</i>												
InsNet (Lu et al., 2022a)	-	-	18.7	-	-	-	-	-	100.0	-	100.0	-
NeuroLogic (Lu et al., 2021)	-	41.9	-	24.7	-	14.4	-	27.5	-	96.7	-	-
A*esque (Lu et al., 2022b)	-	44.3	-	28.6	-	15.6	-	29.6	-	97.1	-	-
NADO (Meng et al., 2022)	-	-	26.2	-	-	-	-	-	96.1	-	-	-
GeLaTo	44.6	44.1	29.9	29.4	16.0	15.8	31.3	31.0	100.0	100.0	100.0	100.0

Step 2: Control p_{gpt} via p_{hmm}

Supervised

Language model is fine-tuned to perform constrained generation (e.g. seq2seq)

Empirically $p_{HMM}(\alpha | x_{1:t+1}) \approx p_{gpt}(\alpha | x_{1:t+1})$ does not hold well enough;

we view $p_{HMM}(x_{t+1} | x_{1:t}, \alpha)$ and $p_{gpt}(x_{t+1} | x_{1:t})$ as classifiers trained for the same task with different biases; thus we generate from their weighted geometric mean:

$$p(x_{t+1} | x_{1:t}, \alpha) \propto p_{hmm}(x_{t+1} | x_{1:t}, \alpha)^w \cdot p_{gpt}(x_{t+1} | x_{1:t})^{1-w}$$

Method	Generation Quality								Constraint Satisfaction			
	ROUGE-L		BLEU-4		CIDEr		SPICE		Coverage		Success Rate	
<i>Supervised</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>	<i>dev</i>	<i>test</i>
NeuroLogic (Lu et al., 2021)	-	42.8	-	26.7	-	14.7	-	30.5	-	97.7	-	93.9 [†]
A*esque (Lu et al., 2022b)	-	43.6	-	28.2	-	15.2	-	30.8	-	97.8	-	97.9 [†]
NADO (Meng et al., 2022)	44.4 [†]	-	30.8	-	16.1 [†]	-	32.0[†]	-	97.1	-	88.8 [†]	-
GeLaTo	46.0	45.6	34.1	32.9	16.7	16.8	31.3	31.9	100.0	100.0	100.0	100.0

Advantages of GeLaTo:

1. Constraint α is guaranteed to be satisfied: for any next-token x_{t+1} that would make α unsatisfiable, $p(x_{t+1} | x_{1:t}, \alpha) = 0$ for both settings.
2. Training p_{hmm} does not depend on α , which is only imposed at inference (generation) time. Once p_{hmm} is trained, we can impose whatever α .
3. We can impose additional tractable constraints:
 - The keywords are generated following a particular order.
 - (Some) keywords must appear at a particular position.
 - (Some) keywords must not appear in the generated sentence.

Conclusion: you can control an intractable generative model using a tractable probabilistic circuit.

Smoothness + ***decomposability*** = ***tractable MAP***

We can also decompose bottom-up a MAP query:

$$\max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e})$$

Smoothness + **decomposability** = ~~tractable MAP~~

We **cannot** decompose bottom-up a MAP query:

$$\max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e})$$

since for a sum node we are marginalizing out a latent variable

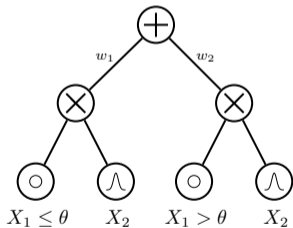
$$\max_{\mathbf{q}} \sum_i w_i p_i(\mathbf{q}, \mathbf{e}) = \max_{\mathbf{q}} \sum_{\mathbf{z}} p(\mathbf{q}, \mathbf{z}, \mathbf{e}) \neq \sum_{\mathbf{z}} \max_{\mathbf{q}} p(\mathbf{q}, \mathbf{z}, \mathbf{e})$$

\Rightarrow MAP for latent variable models is **intractable** (Conaty et al. 2017)

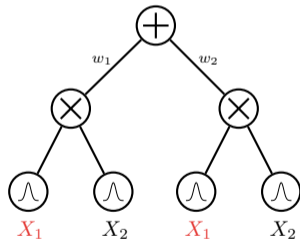
Determinism

aka selectivity

A sum node is deterministic if the output of only one children is non zero for any input
 \Rightarrow e.g. if their distributions have disjoint support



deterministic circuit



non-deterministic circuit

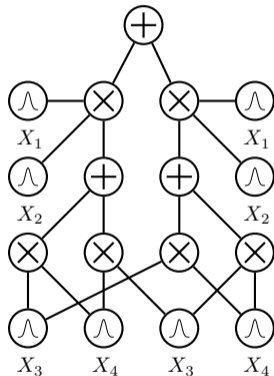
Determinism + **decomposability** = **tractable MAP**

Computing maximization with arbitrary evidence e

\Rightarrow *linear in circuit size!*

E.g., suppose we want to compute:

$$\max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e})$$

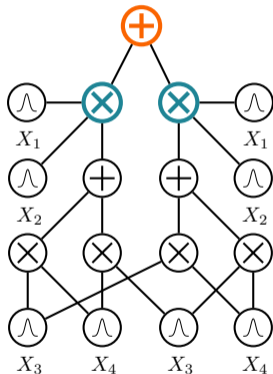


Determinism + decomposability = tractable MAP

If $p(\mathbf{q}, \mathbf{e}) = \sum_i w_i p_i(\mathbf{q}, \mathbf{e}) = \max_i w_i p_i(\mathbf{q}, \mathbf{e})$,
 (**deterministic** sum node):

$$\begin{aligned} \max_{\mathbf{q}} p(\mathbf{q}, \mathbf{e}) &= \max_{\mathbf{q}} \sum_i w_i p_i(\mathbf{q}, \mathbf{e}) \\ &= \max_{\mathbf{q}} \max_i w_i p_i(\mathbf{q}, \mathbf{e}) \\ &= \max_i \max_{\mathbf{q}} w_i p_i(\mathbf{q}, \mathbf{e}) \end{aligned}$$

⇒ *one non-zero child term, thus sum is max*

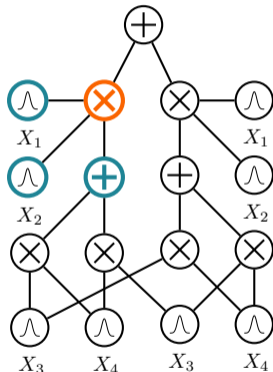


Determinism + **decomposability** = **tractable MAP**

If $p(\mathbf{q}, \mathbf{e}) = p(\mathbf{q}_x, \mathbf{e}_x, \mathbf{q}_y, \mathbf{e}_y) = p(\mathbf{q}_x, \mathbf{e}_x)p(\mathbf{q}_y, \mathbf{e}_y)$
 (**decomposable** product node):

$$\begin{aligned} \max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e}) &= \max_{\mathbf{q}} p(\mathbf{q}, \mathbf{e}) \\ &= \max_{\mathbf{q}_x, \mathbf{q}_y} p(\mathbf{q}_x, \mathbf{e}_x, \mathbf{q}_y, \mathbf{e}_y) \\ &= \max_{\mathbf{q}_x} p(\mathbf{q}_x, \mathbf{e}_x) \cdot \max_{\mathbf{q}_y} p(\mathbf{q}_y, \mathbf{e}_y) \end{aligned}$$

\Rightarrow solving optimization independently



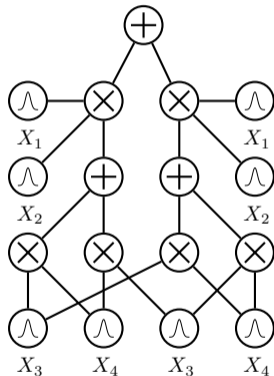
Determinism + **decomposability** = **tractable MAP**

Evaluating the circuit twice:

bottom-up and **top-down**



still linear in circuit size!



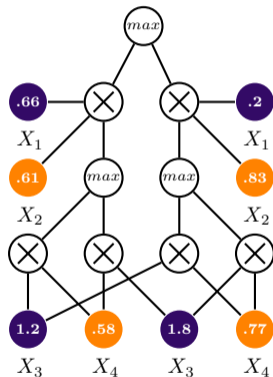
Determinism + decomposability = tractable MAP

Evaluating the circuit twice:

bottom-up and **top-down** \Rightarrow still linear in circuit size!

E.g., for $\operatorname{argmax}_{x_1, x_3} p(x_1, x_3 \mid x_2, x_4)$:

1. turn sum into max nodes and distributions into max distributions
2. evaluate $p(x_2, x_4)$ bottom-up
3. retrieve max activations top-down
4. compute **MAP states** for X_1 and X_3 at leaves



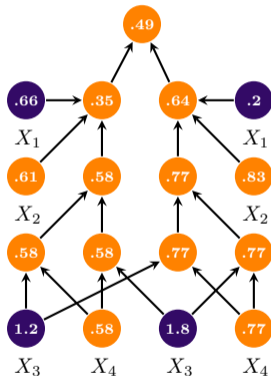
Determinism + **decomposability** = **tractable MAP**

Evaluating the circuit twice:

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E.g., for $\operatorname{argmax}_{x_1, x_3} p(x_1, x_3 \mid x_2, x_4)$:

1. turn sum into max nodes and distributions into max distributions
2. evaluate $p(x_2, x_4)$ bottom-up
3. retrieve max activations top-down
4. compute **MAP states** for X_1 and X_3 at leaves



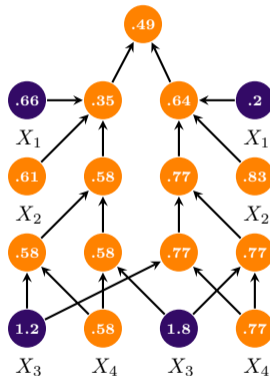
Determinism + **decomposability** = **tractable MAP**

Evaluating the circuit twice:

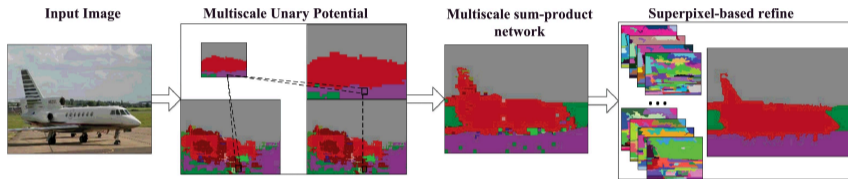
bottom-up and **top-down** \Rightarrow *still linear in circuit size!*

E.g., for $\operatorname{argmax}_{x_1, x_3} p(x_1, x_3 \mid x_2, x_4)$:

1. turn sum into max nodes and distributions into max distributions
2. evaluate $p(x_2, x_4)$ bottom-up
3. retrieve max activations top-down
4. compute **MAP states** for X_1 and X_3 at leaves



MAP inference : image segmentation



Semantic segmentation is MAP over joint pixel and label space

Even approximate MAP for non-deterministic circuits (SPNs) delivers good performances.

Rathke et al., "Locally adaptive probabilistic models for global segmentation of pathological oct scans", 2017

Yuan et al., "Modeling spatial layout for scene image understanding via a novel multiscale sum-product network", 2016

Friesen and Domingos, "Submodular Sum-product Networks for Scene Understanding", 2016

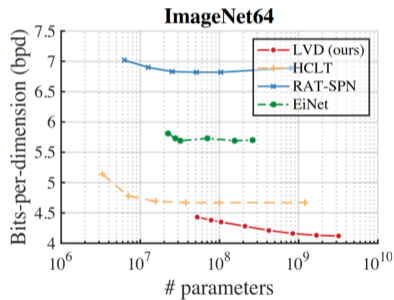
How expressive?

Dataset	Sparse PC (ours)	HCLT	RatSPN	IDF	BitSwap	BB-ANS	McBits
MNIST	1.14	1.20	1.67	1.90	1.27	1.39	1.98
EMNIST(MNIST)	1.52	1.77	2.56	2.07	1.88	2.04	2.19
EMNIST(Letters)	1.58	1.80	2.73	1.95	1.84	2.26	3.12
EMNIST(Balanced)	1.60	1.82	2.78	2.15	1.96	2.23	2.88
EMNIST(ByClass)	1.54	1.85	2.72	1.98	1.87	2.23	3.14
FashionMNIST	3.27	3.34	4.29	3.47	3.28	3.66	3.72

competitive with Flows and VAEs!

How scalable?

Dataset	TPMs				DGMs		
	LVD (ours)	HCLT	EiNet	RAT-SPN	Glow	RealNVP	BIVA
ImageNet32	4.39 \pm 0.01	4.82	5.63	6.90	4.09	4.28	3.96
ImageNet64	4.12 \pm 0.00	4.67	5.69	6.82	3.81	3.98	-
CIFAR	4.38 \pm 0.02	4.61	5.81	6.95	3.35	3.49	3.08



up to billions of parameters

Questions answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
3. ***What is the connection to logical circuit languages?*** (YooJung)
4. *How do I compile my favorite model into a circuit?* (YooJung)
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Logical Circuits

Tractability to other semi-rings

Tractable probabilistic inference exploits **efficient summation for decomposable functions** in the probability commutative semiring:

$$(\mathbb{R}, +, \times, 0, 1)$$

analogously efficient computations can be done in other semi-rings:

$$(\mathbb{S}, \oplus, \otimes, 0_{\oplus}, 1_{\otimes})$$

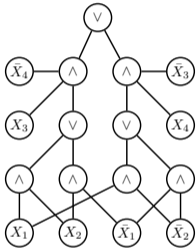
\Rightarrow Algebraic model counting (Kimmig et al. 2017), Semi-ring programming (Belle et al. 2016)

Historically, **very well studied for boolean functions**:

$$(\mathbb{B} = \{0, 1\}, \vee, \wedge, 0, 1)$$

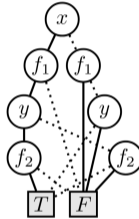
\Rightarrow logical circuits!

Logical circuits



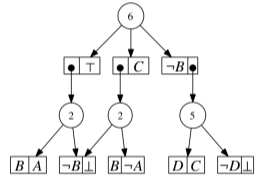
s/d-D/NNFs

(Darwiche et al. 2002a)



O/BDDs

(Bryant 1986)



SDDs

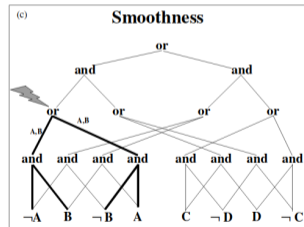
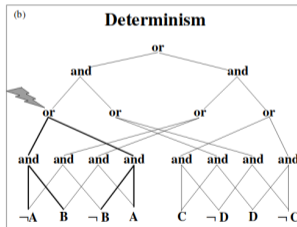
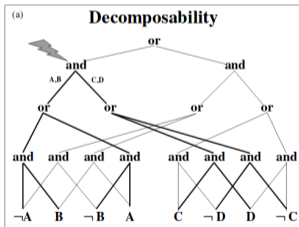
(Darwiche 2011a)

Logical circuits are compact representations for boolean functions...

Logical circuits

structural properties

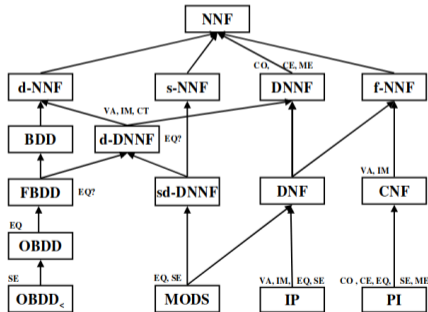
...and like probabilistic circuits, one can define **structural properties**: (structured) decomposability, smoothness, determinism allowing for tractable computations



Logical circuits

a knowledge compilation map

...inducing a **hierarchy of tractable logical circuit families**

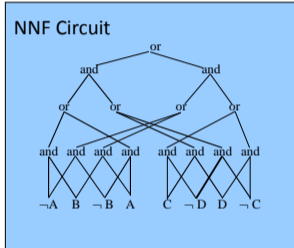


Knowledge Compilation

encoding

```
(A and (not B))  
or(C and (not D))  
or ((not C) and D)  
...
```

Compiler

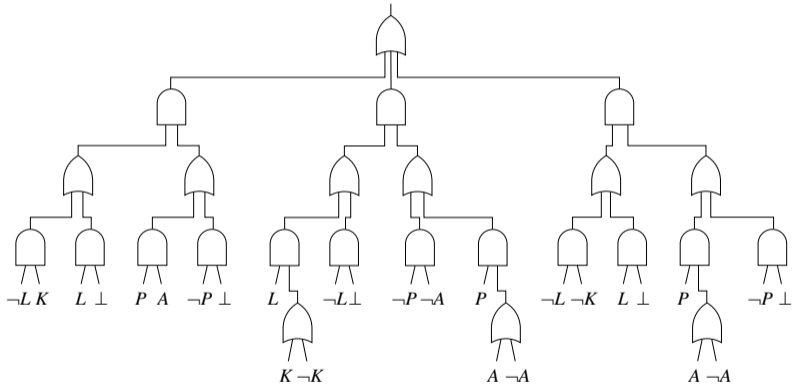


MAJ-MAJ-SAT
E-MAJ-SAT
MAJ-SAT
SAT

**Answer in
Linear Time**

NNF Circuits

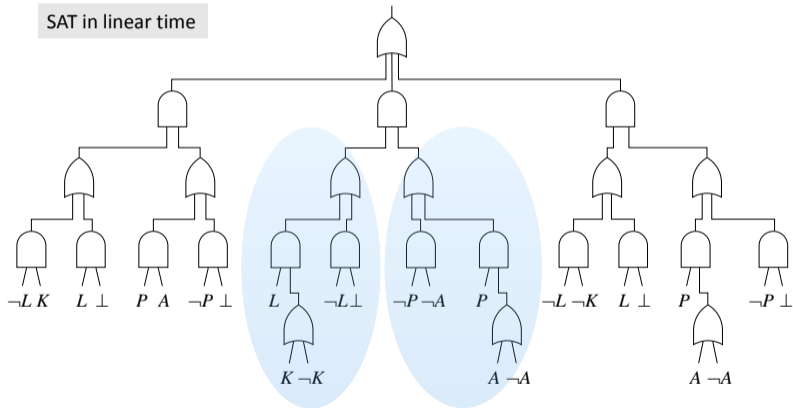
$$P \vee L$$
$$A \Rightarrow P$$
$$K \Rightarrow (P \vee L)$$



Decomposability (DNNF)

Darwiche, JACM 2001

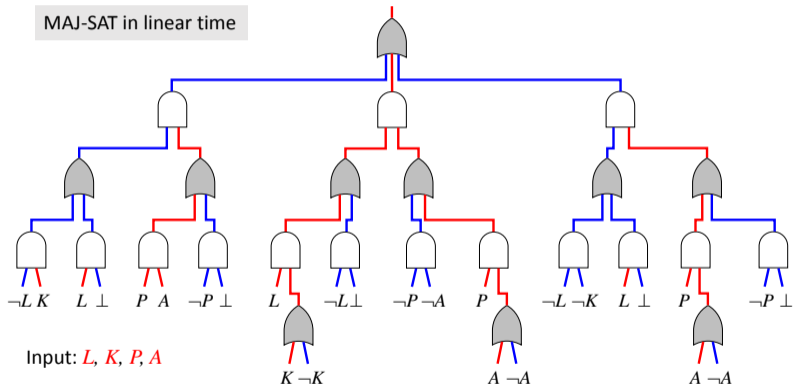
SAT in linear time



Determinism (d-DNNF)

Darwiche, JANCL 2000

MAJ-SAT in linear time



Decomposability + **determinism** = **tractable (W)MC**

Model counting problem: given a Boolean formula Δ , compute the number of satisfying assignments.

Weighted model counting (WMC):

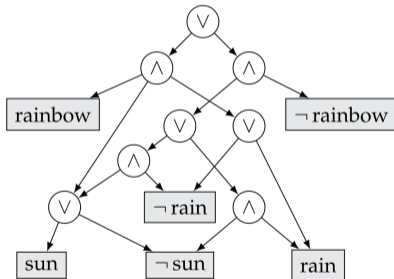
$$\text{WMC}(\Delta, w) = \sum_{\mathbf{x} \models \Delta} \prod_{l \in \mathbf{x}} w(l)$$

\Rightarrow *linear in circuit size!*

Decomposability + **determinism** = **tractable (W)MC**

To compute $WMC(\Delta, w)$:

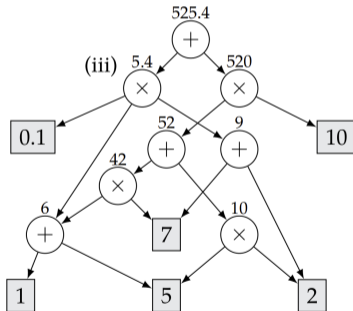
- Turn OR gates to sum nodes and AND gates to product nodes
- Replace each literal l with its weight $w(l)$
- bottom-up evaluation



Decomposability + **determinism** = **tractable (W)MC**

To compute $WMC(\Delta, w)$:

- Turn OR gates to sum nodes and AND gates to product nodes
- Replace each literal l with its weight $w(l)$
- bottom-up evaluation



Probabilistic inference by WMC

connection to probabilistic circuits through WMC

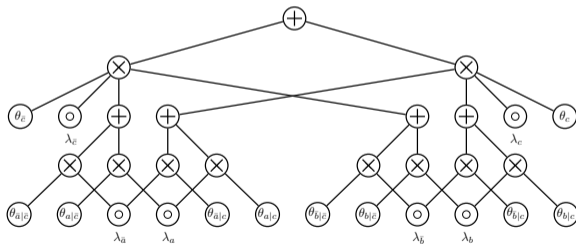
1. Encode probabilistic model as WMC formula (Δ, w)
2. Compile Δ into a logical circuit (e.g. d-DNNF, OBDD, SDD, etc.)
3. Tractable MAR/CON by tractable WMC on circuit
4. Answer *complex queries* tractably by enforcing *more structural properties!*

Probabilistic inference by WMC

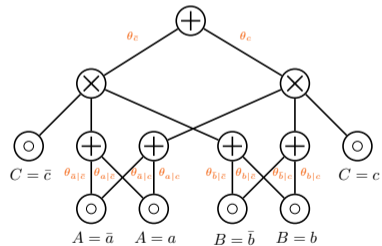
connection to probabilistic circuits through WMC

Resulting compiled WMC circuit **equivalent to probabilistic circuit**

\Rightarrow parameter variables \rightarrow edge parameters



Compiled circuit of WMC encoding



Equivalent probabilistic circuit

Questions answered today

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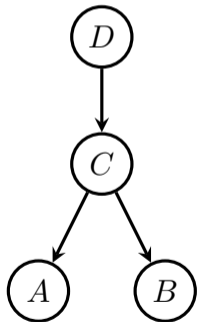
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From tree BN to circuits

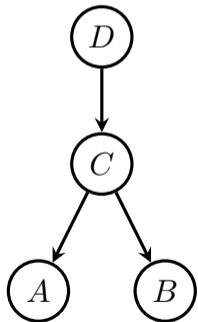
via compilation

Bottom-up **compilation**: starting from leaves...



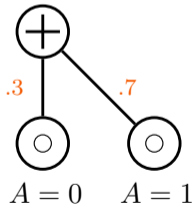
From tree BN to circuits

via compilation



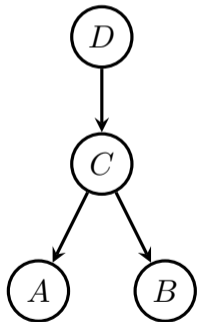
...compile a leaf CPT

$p(A|C = 0)$

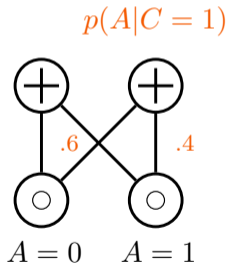


From tree BN to circuits

via compilation

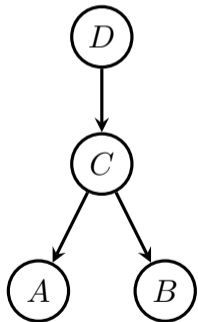


...compile a leaf CPT

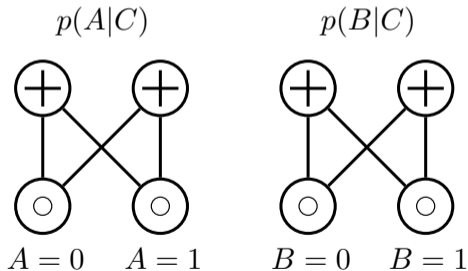


From tree BN to circuits

via compilation



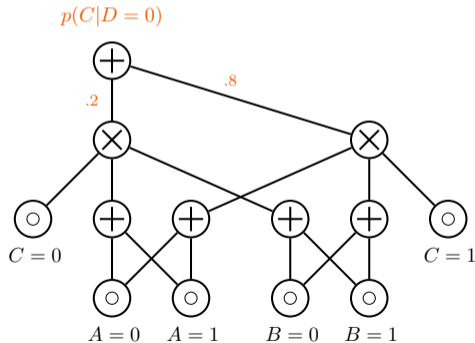
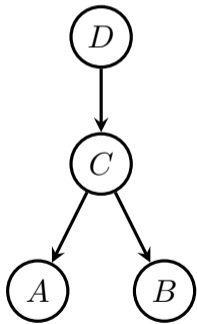
...compile a leaf CPT...for all leaves...



From tree BN to circuits

via compilation

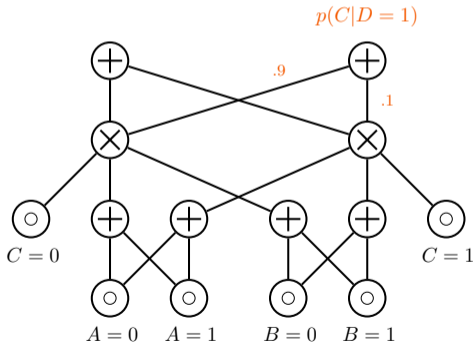
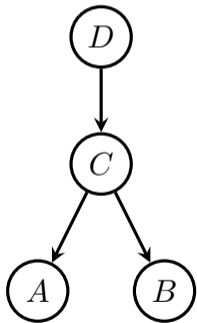
...and recurse over parents...



From tree BN to circuits

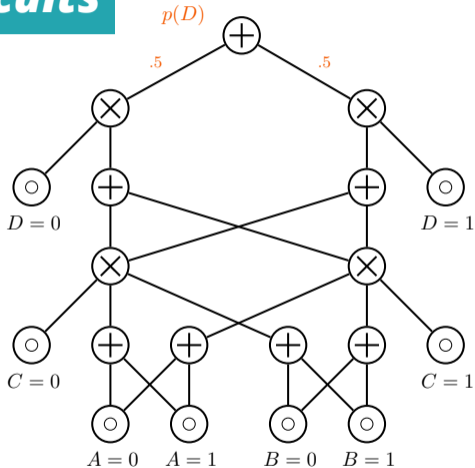
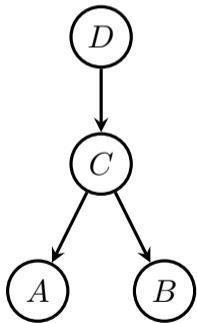
via compilation

...while reusing previously compiled nodes!...



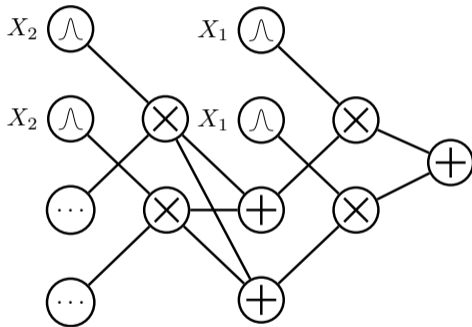
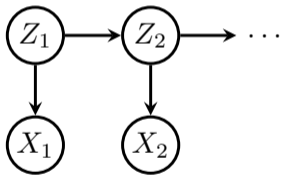
From tree BN to circuits

via compilation



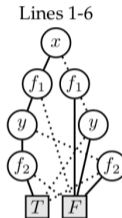
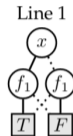
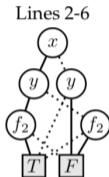
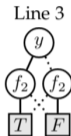
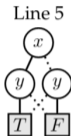
Hidden Markov Models

as computational graphs



Compilation : probabilistic programming

```
1 x = flip( $\theta_1$ );  
2 if(x) {  
3   y = flip( $\theta_2$ )  
4 } else {  
5   y = x  
6 }
```



Chavira et al., "Compiling relational Bayesian networks for exact inference", 2006

Holtzen et al., "Symbolic Exact Inference for Discrete Probabilistic Programs", 2019

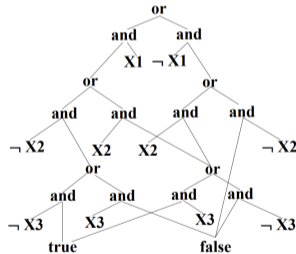
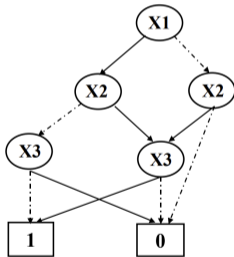
De Raedt et al.; Riguzzi; Fierens et al.; Vlasselaer et al., "ProbLog: A Probabilistic Prolog and Its Application in Link Discovery."; "A top down interpreter for LPAD and CP-logic"; "Inference and Learning in Probabilistic Logic Programs using Weighted Boolean Formulas"; "Anytime Inference in Probabilistic Logic Programs with Tp-compilation", 2007; 2007; 2015; 2015

Olteanu et al.; Van den Broeck et al., "Using OBDDs for efficient query evaluation on probabilistic databases"; Query Processing on Probabilistic Data: A Survey, 2008; 2017

Vlasselaer et al., "Exploiting Local and Repeated Structure in Dynamic Bayesian Networks", 2016

Decision Diagrams

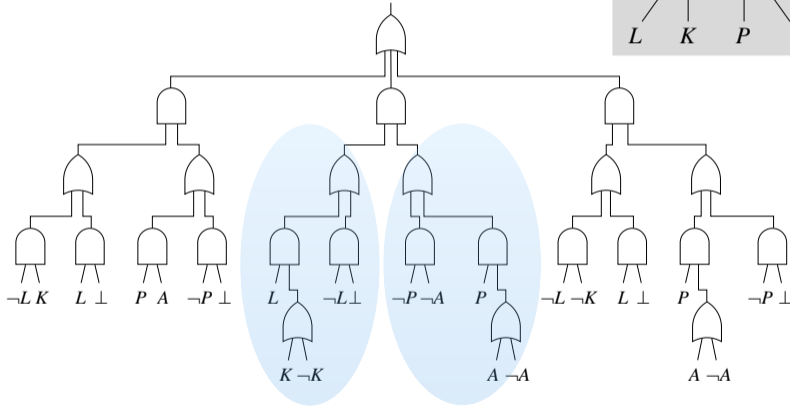
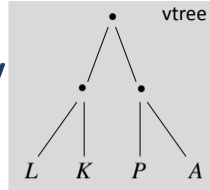
- FBDDs (Free binary decision diagrams; *read-once*)
- OBDDs (Ordered Binary Decision Diagrams)
- SDDs (Sentential decision diagrams)



⇒ BDD as circuit

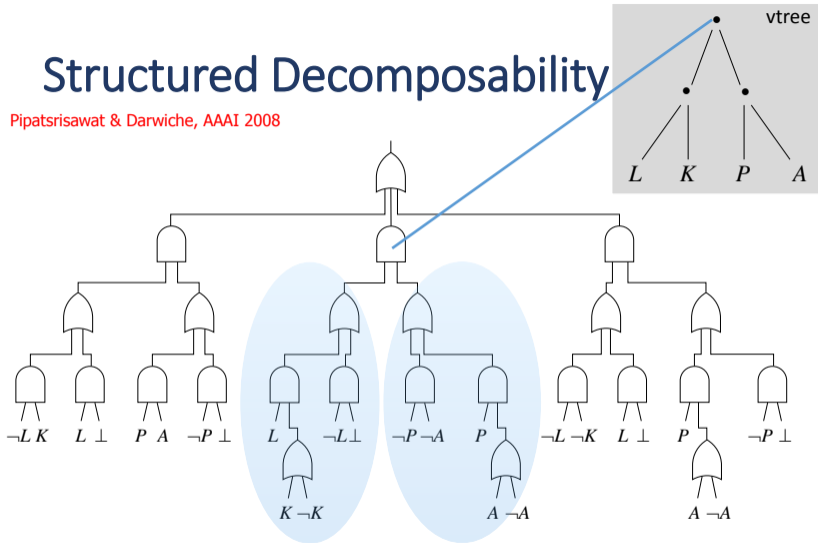
Structured Decomposability

Pipatsrisawat & Darwiche, AAI 2008



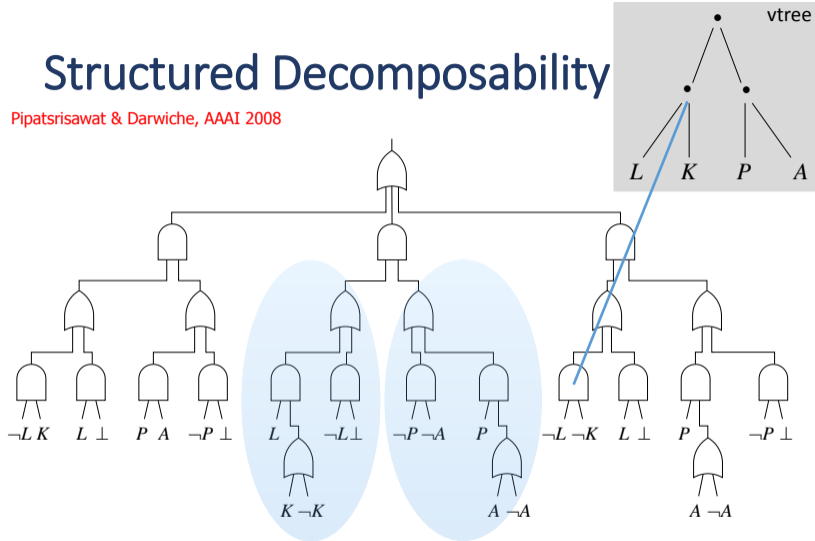
Structured Decomposability

Pipatsrisawat & Darwiche, AAAI 2008



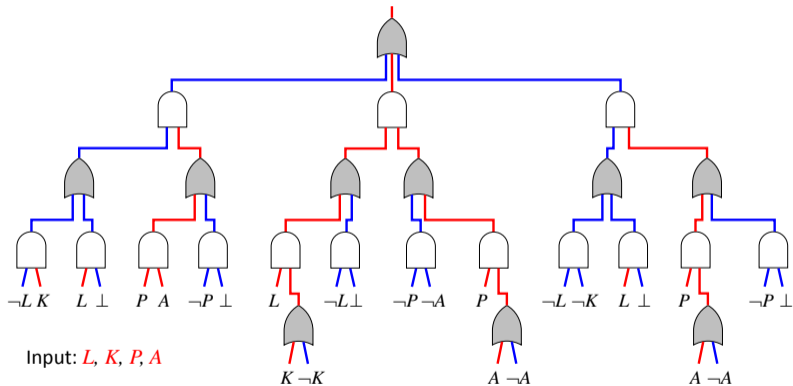
Structured Decomposability

Pipatsrisawat & Darwiche, AAI 2008



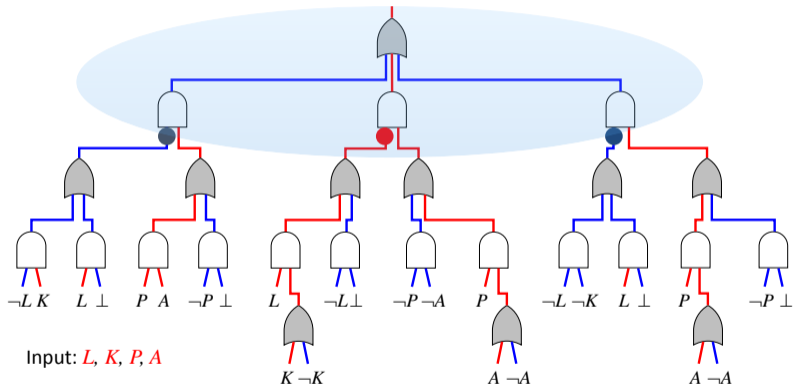
Partitioned Determinism (SDDs)

Darwiche, IJCAI 2011



Partitioned Determinism (SDDs)

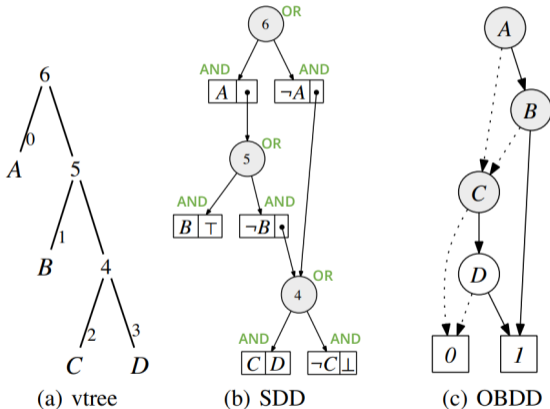
Darwiche, IJCAI 2011



Decision Diagrams

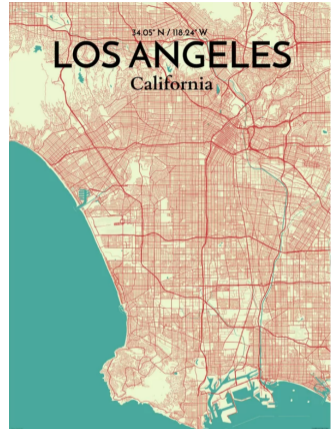
- FBDDs (Free binary decision diagrams; *read-once*)
- OBDDs (Ordered BDDs)
- SDDs (Sentential decision diagrams)

\Rightarrow SDD & OBDD for $(A \wedge B) \vee (C \wedge D)$



Probability of logical events

q₈: *What is the probability of having a traffic jam on my route to campus?*



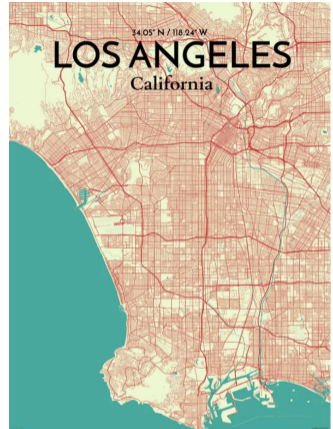
© fineartamerica.com

Probability of logical events

q_8 : What is the probability of having a traffic jam on my route to campus?

$$q_8(\mathbf{m}) = p_{\mathbf{m}}(\bigvee_{i \in \text{route}} \text{Jam}_{\text{Str } i})$$

\Rightarrow *marginals + logical events*



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Smoothness + **structured decomp.** = **tractable PR**

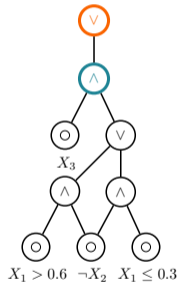
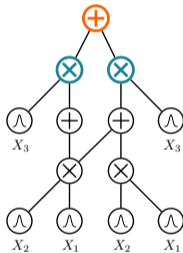
If $p(\mathbf{x}) = \sum_i w_i p_i(\mathbf{x})$, $\alpha = \bigvee_j \alpha_j$,

(smooth p)

(smooth + deterministic α):

$$p(\alpha) = \sum_i w_i p_i \left(\bigvee_j \alpha_j \right) = \sum_i w_i \sum_j p_i(\alpha_j)$$

\Rightarrow probabilities are "pushed down" to children

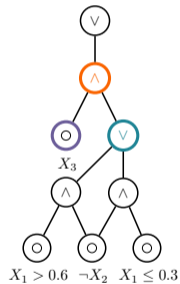
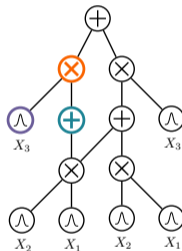


Smoothness + **structured decomp.** = **tractable PR**

If $p(\mathbf{x}, \mathbf{y}) = p(\mathbf{x})p(\mathbf{y})$, $\alpha = \beta \wedge \gamma$,
 (structured decomposability):

$$p(\alpha) = p(\beta \wedge \gamma) \cdot p(\beta \wedge \gamma) = p(\beta) \cdot p(\gamma)$$

\Rightarrow probabilities decompose into simpler ones



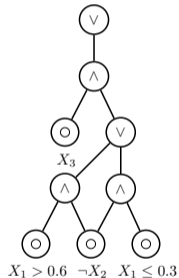
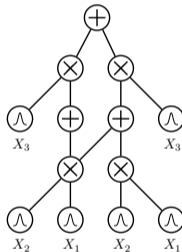
Smoothness + **structured decomp.** = **tractable PR**

To compute $p(\alpha)$:

- compute the probability for each **pair** of probabilistic and logical circuit nodes for the **same vtree node**

\Rightarrow *cache the values!*

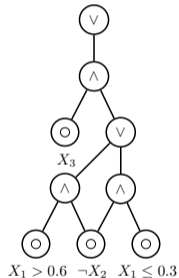
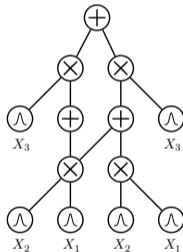
- feedforward evaluation (bottom-up)



Smoothness + **structured decomp.** = **tractable PR**

To compute $p(\alpha)$:

- compute the probability for each **pair** of probabilistic and logical circuit nodes for the **same vtree node**
 \Rightarrow *cache the values!*
- feedforward evaluation (bottom-up)



structured decomposability = **tractable...**

- **Symmetric** and **group queries** (exactly- k , odd-number, etc.) (Bekker et al. 2015)

For the “right” vtree

- Marginal MAP (Oztok et al. 2016)
- Probability of logical circuit event in probabilistic circuit (Choi et al. 2015b)
- **Multiply** two probabilistic circuits (Shen et al. 2016)
- **KL Divergence** between probabilistic circuits (Liang et al. 2017)
- **Same-decision probability** (Oztok et al. 2016)
- **Expected same-decision probability** (Choi et al. 2017)
- **Expected classifier agreement** (Choi et al. 2018)
- **Expected predictions** (Khosravi et al. 2019b)

Questions answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
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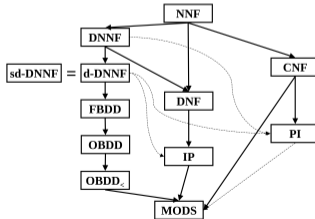
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Succinctness of circuits

Expressive efficiency

Tractability is defined with respect to the size of the model.

How do structural constraints affect **expressive efficiency (succinctness)** of probabilistic/logical circuits?



Succinctness of circuits

Expressive efficiency

A family of circuits \mathcal{M}_1 is **at least as succinct as** \mathcal{M}_2
iff for every $m_2 \in \mathcal{M}_2$, there exists $m_1 \in \mathcal{M}_1$ that represents
the same function and $|m_1| \leq |\text{poly}(m_2)|$.

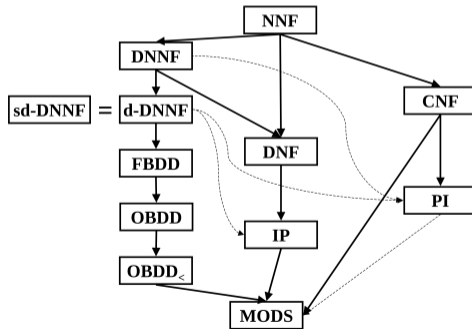
\Rightarrow denoted $\mathcal{M}_1 \leq \mathcal{M}_2$

\Rightarrow strictly more succinct ($\mathcal{M}_1 < \mathcal{M}_2$)
iff $\mathcal{M}_1 \leq \mathcal{M}_2$ and $\mathcal{M}_1 \not\leq \mathcal{M}_2$

Succinctness of circuits

Expressive efficiency

Strict succinctness ordering: DNNF < d-DNNF < FBDD < OBDD



Succinctness of circuits

Expressive efficiency

Strict succinctness ordering: **DNNF** < **d-DNNF** < FBDD < OBDD

- d-DNNF $\not\leq$ DNNF unless the polynomial hierarchy collapses (*Darwiche et al. 2002a*).
- The *Sauerhoff function* has DNNF of size $O(n^2)$ but d-DNNF of size $2^{\Omega(n)}$ (*Bova et al. 2016*).

Succinctness of circuits

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\Rightarrow Unconditional exponential separation for d-DNNF $\not\leq$ DNNF

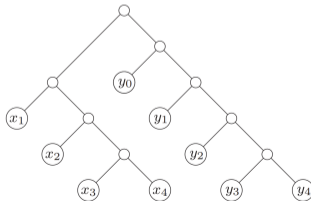
\Rightarrow Using a connection between circuits
and **communication complexity**

Succinctness of circuits

Expressive efficiency

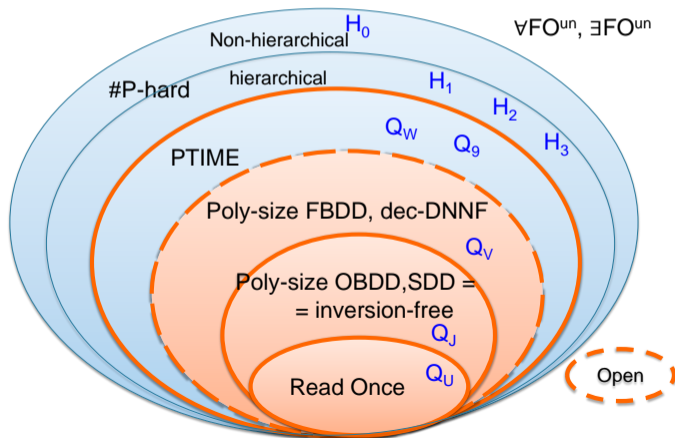
SDD < OBDD: SDDs are strictly more succinct than OBDDs

- $SDD \leq OBDD$: OBDDs are SDDs with right-linear vtrees
- $SDD \not\leq OBDD$: The *hidden weighted bit function* has SDD of size $O(n^3)$ but OBDD of size $2^{\Omega(n)}$.



Query compilation

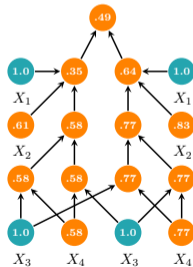
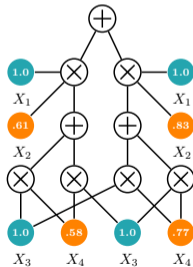
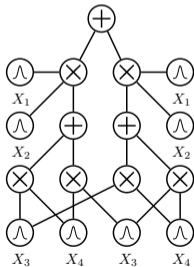
Möbius Über Alles



***How precise is the characterization
of tractable circuits
by structural properties?***

Smoothness + **decomposability** = **tractable MAR**

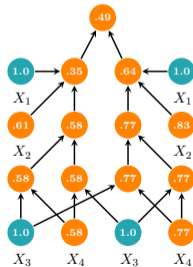
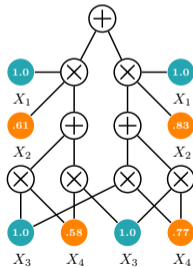
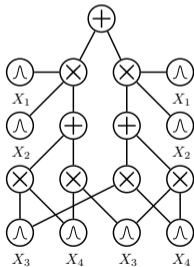
Recall: Smoothness and decomposability allow marginal inference by feedforward (sum-product) evaluation.



Smoothness + **decomposability** = **tractable MAR**

Recall: Smoothness and decomposability allow marginal inference by feedforward (sum-product) evaluation.

⇒ Are these properties necessary?

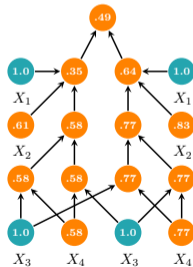
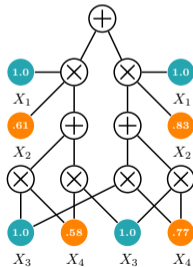
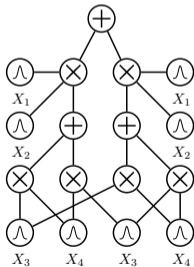


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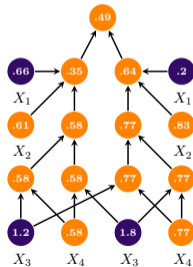
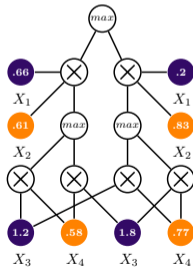
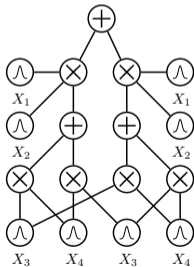
⇒ Are these properties necessary?

⇒ Yes! Otherwise, integrals do not decompose.



Determinism + **decomposability** = **tractable MAP**

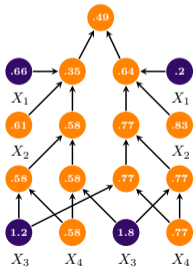
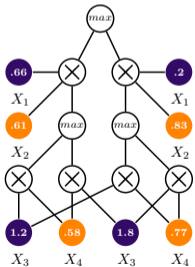
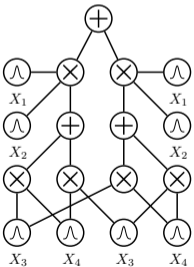
Recall: Determinism and decomposability allow MAP inference by feedforward (max-product) evaluation.



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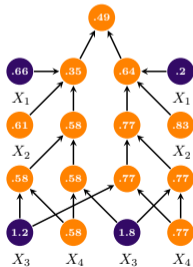
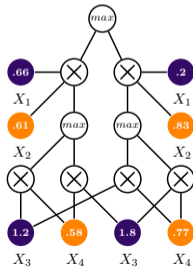
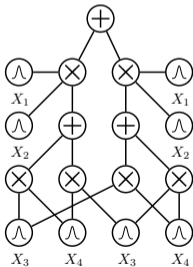
⇒ However, decomposability is not necessary!



Determinism + **decomposability** = **tractable MAP**

Recall: Determinism and decomposability allow MAP inference by feedforward (max-product) evaluation.

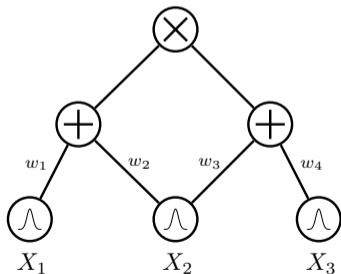
⇒ However, decomposability is not necessary!
 ⇒ A weaker condition, **consistency**, suffices.



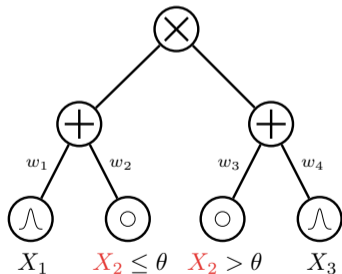
Consistency

A product node is consistent if any variable shared between its children appears in a single leaf node

\Rightarrow decomposability implies consistency



consistent circuit



inconsistent circuit

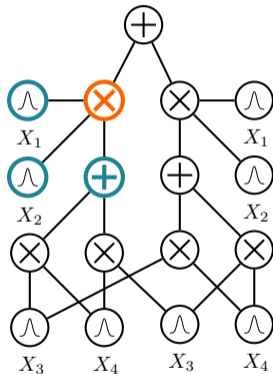
Determinism + ***consistency*** = ***tractable MAP***

Determinism + consistency = tractable MAP

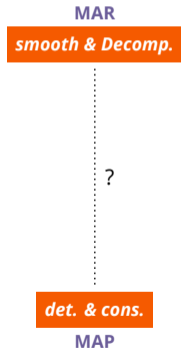
If $\max_{\mathbf{q}_{\text{shared}}} p(\mathbf{q}, \mathbf{e}) =$
 $\max_{\mathbf{q}_{\text{x}}} p(\mathbf{q}_{\text{x}}, \mathbf{e}_{\text{x}}) \cdot \max_{\mathbf{q}_{\text{y}}} p(\mathbf{q}_{\text{y}}, \mathbf{e}_{\text{y}})$ (**consistent**):

$$\begin{aligned} \max_{\mathbf{q}} p(\mathbf{q}, \mathbf{e}) &= \max_{\mathbf{q}_{\text{x}}, \mathbf{q}_{\text{y}}} p(\mathbf{q}_{\text{x}}, \mathbf{e}_{\text{x}}, \mathbf{q}_{\text{y}}, \mathbf{e}_{\text{y}}) \\ &= \max_{\mathbf{q}_{\text{x}}} p(\mathbf{q}_{\text{x}}, \mathbf{e}_{\text{x}}) \cdot \max_{\mathbf{q}_{\text{y}}} p(\mathbf{q}_{\text{y}}, \mathbf{e}_{\text{y}}) \end{aligned}$$

\Rightarrow solving optimization independently

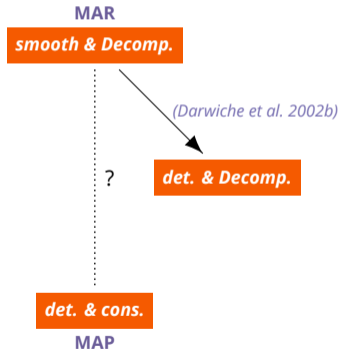


Expressive efficiency of circuits



Are smooth & decomposable circuits as succinct as deterministic & consistent ones, or vice versa?

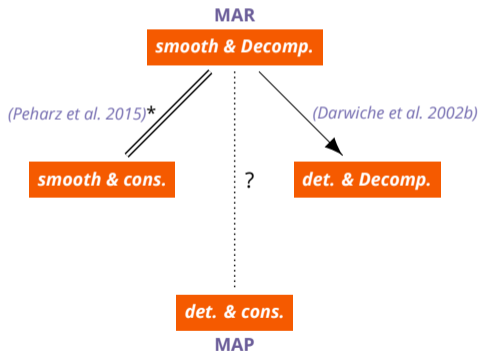
Expressive efficiency of circuits



- Smooth & decomposable circuits strictly more succinct than deterministic & decomposable ones
- Smooth & consistent circuits are equally succinct as smooth & decomposable ones

→ : strictly more succinct

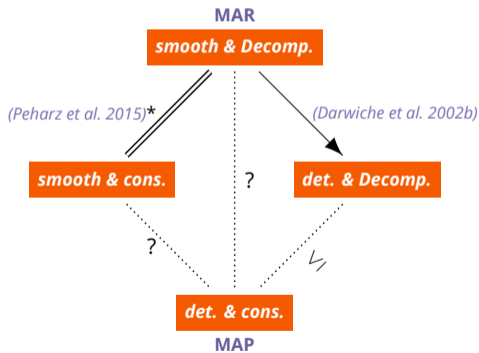
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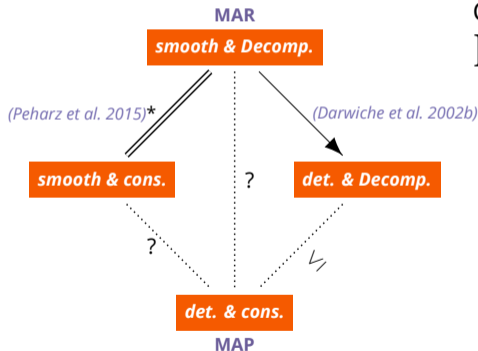
Expressive efficiency of circuits



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Expressive efficiency of circuits



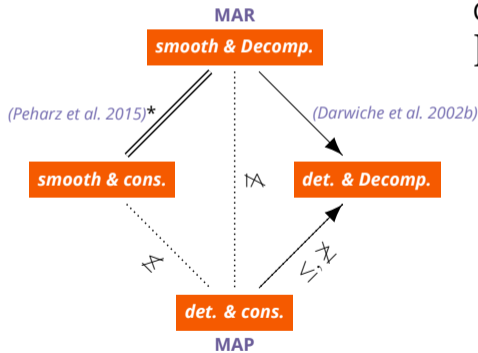
→ : strictly more succinct
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Consider following circuit over Boolean variables:

$$\prod_i^r (Y_i \cdot Z_{i1} + (\neg Y_i) \cdot Z_{i2}), \quad Z_{ij} \in \mathbf{X}$$

- Size linear in the number of variables
- Deterministic and consistent
- Marginal (with no evidence) is the solution to #P-hard SAT' problem (Valiant 1979) \Rightarrow **no tractable circuit for marginals!**

Expressive efficiency of circuits



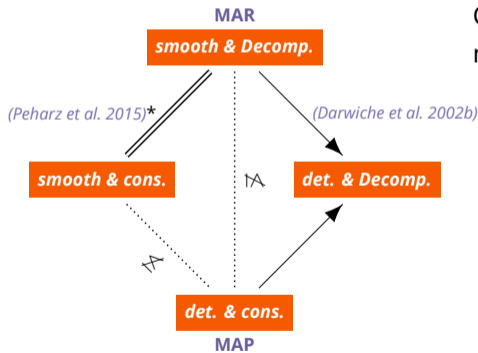
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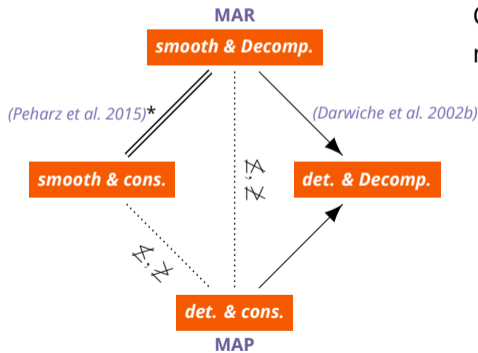


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Consider the marginal distribution $p(\mathbf{X})$ from a naive Bayes distribution $p(\mathbf{X}, C)$:

- Linear-size smooth and decomposable circuit
- MAP of $p(\mathbf{X})$ solves marginal MAP of $p(\mathbf{X}, C)$ which is NP-hard (*de Campos 2011*)
 \Rightarrow **no tractable circuit for MAP!**

Expressive efficiency of circuits

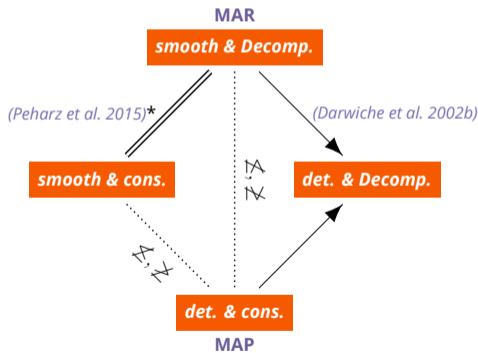


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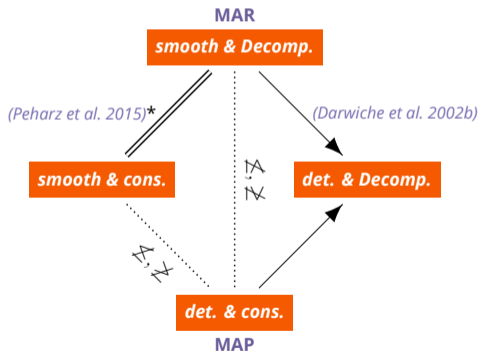
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Neither smooth & decomposable nor deterministic & consistent circuits are more succinct than the other!

⇒ Choose tractable circuit family based on your query

More theoretical questions remaining
⇒ "Complete the map"

Expressive efficiency of circuits



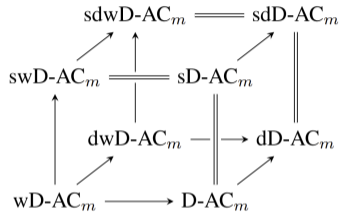
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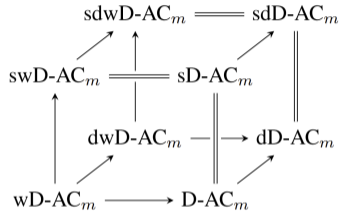
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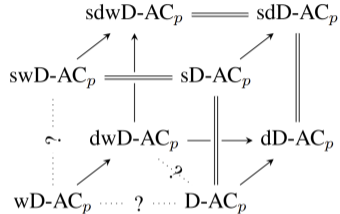
Succinctness map for *monotone* circuits

\Rightarrow (s)mooth, (d)eterministic, (D)ecomposable, (w)eak (D)ecomposable (i.e. consistent)

Expressive efficiency of circuits



Succinctness map for *monotone* circuits



Succinctness map for *positive* circuits
(non-negative output, but weights may be negative)

\Rightarrow (s)mooth, (d)eterministic, (D)ecomposable, (w)eak (D)ecomposable (i.e. consistent)

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Goal

***Given a class of queries
can we systematically find
a class of probabilistic circuits
that is tractable for it?***

A language for queries

Integral expressions that can be formed by composing these operators

+, **×**, **pow**, **log**, **exp** and **/**

\Rightarrow *many divergences and information-theoretic queries*

A language for queries

Integral expressions that can be formed by composing these operators

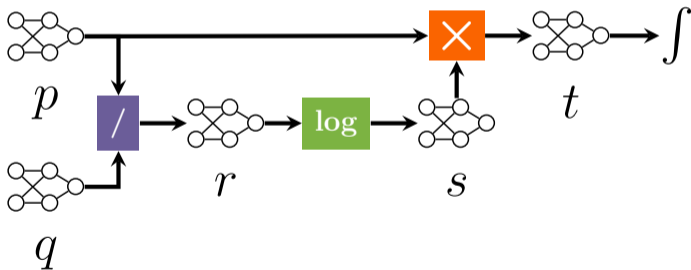
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⇒ *many divergences and information-theoretic queries*

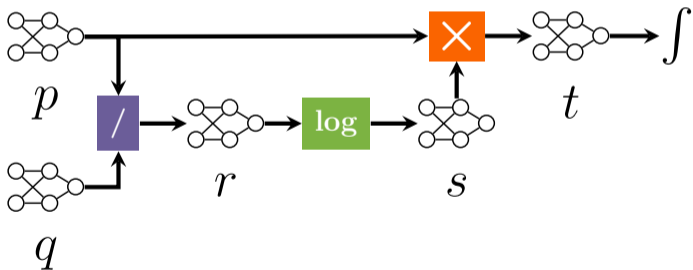
Represented as **higher-order computational graphs**—pipelines—operating over circuits!

⇒ *re-using intermediate transformations across queries*

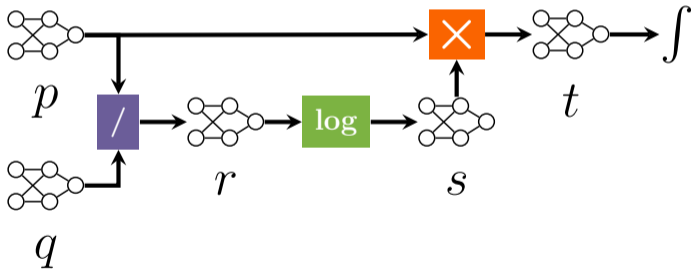
$$\text{KLD}(p \parallel q) = \int_{\text{val}(\mathbf{X})} p(\mathbf{x}) \times \log(p(\mathbf{x})/q(\mathbf{x})) d\mathbf{X}$$



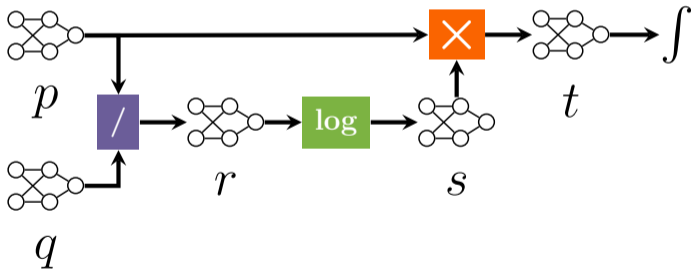
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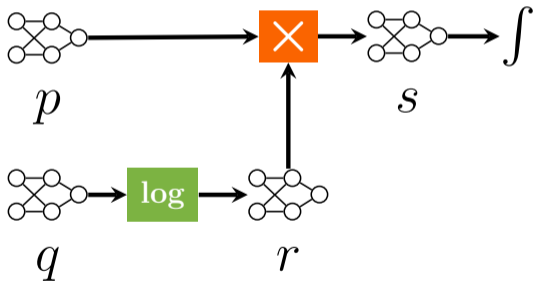
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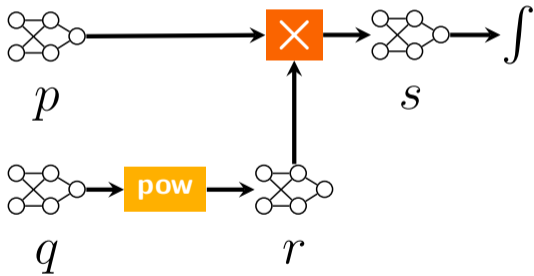
$$\text{KLD}(p \parallel q) = \int_{\text{val}(\mathbf{X})} p(\mathbf{x}) \times \log(p(\mathbf{x})/q(\mathbf{x})) d\mathbf{X}$$



$$\text{XENT}(p \parallel q) = \int p(\mathbf{x}) \times \log q(\mathbf{x}) d\mathbf{X}$$

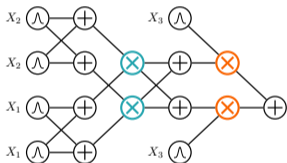


$$\mathbb{E}_{\mathbf{x}^m \sim p(\mathbf{x}^m | \mathbf{x}^o)} [q^\alpha(\mathbf{x}^m, \mathbf{x}^o)]$$

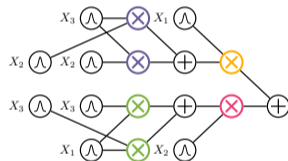


Compatibility

Two circuits are *compatible* if they have the same *hierarchical scope partitioning*
 \Rightarrow generalizes “structured decomposability with same vtree”

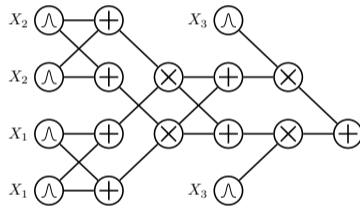
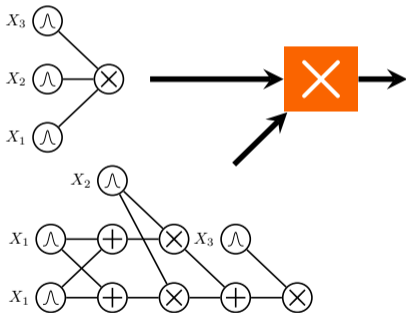


compatible circuits



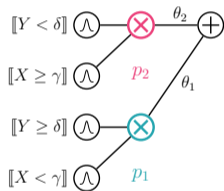
non-compatible circuits

Tractable operators



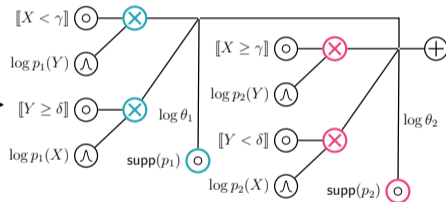
***smooth, decomposable
compatible***

Tractable operators



**smooth, decomposable
deterministic**

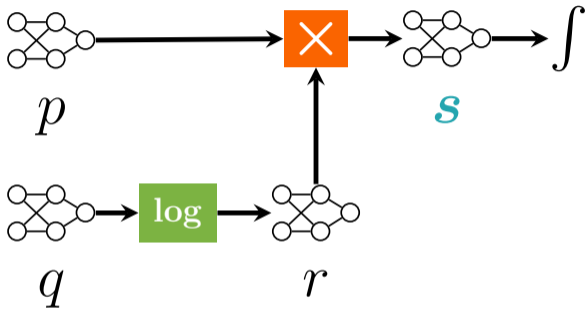
log



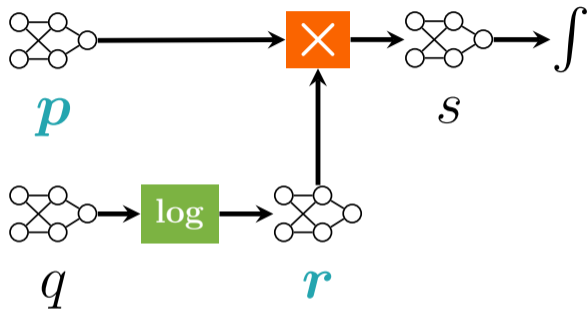
smooth, decomposable

		\times	$p + q$ +	$p \times q$ pow _N	p^n pow _R	p^α /	p/q log	$\log p$ exp
smoothness	SMO	✗	✓	✓	✓	✓	✓	✓
decomposability	DEC	✗	✗	✗	✓	✗	✗	✗
determinism	DET	✗	✗	✗	✓	✓	✓	✗
compatibility	CMP	✗	✓	✓	✗	✓	✗	✗

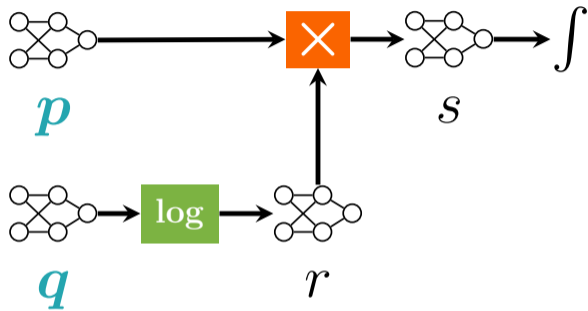
Building an atlas of composable **tractable atomic operations**



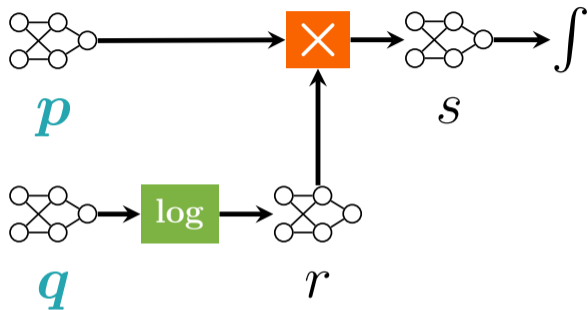
To perform tractable integration we need s to be *smooth and decomposable*...



hence we need p and r to be smooth, decomposable and **compatible**...



therefore q must be smooth, decomposable and **deterministic**...



we can compute XENT tractably if p and q are smooth, decomposable, compatible and q is deterministic...

	Query	Tract. Conditions	Hardness
CROSS ENTROPY	$-\int p(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{X}$	Cmp, q Det	#P-hard w/o Det
SHANNON ENTROPY	$-\sum p(\mathbf{x}) \log p(\mathbf{x})$	Sm, Dec, Det	coNP-hard w/o Det
RÉNYI ENTROPY	$(1 - \alpha)^{-1} \log \int p^\alpha(\mathbf{x}) d\mathbf{X}, \alpha \in \mathbb{N}$	SD	#P-hard w/o SD
	$(1 - \alpha)^{-1} \log \int p^\alpha(\mathbf{x}) d\mathbf{X}, \alpha \in \mathbb{R}_+$	Sm, Dec, Det	#P-hard w/o Det
MUTUAL INFORMATION	$\int p(\mathbf{x}, \mathbf{y}) \log(p(\mathbf{x}, \mathbf{y}) / (p(\mathbf{x})p(\mathbf{y})))$	Sm, SD, Det*	coNP-hard w/o SD
KULLBACK-LEIBLER DIV.	$\int p(\mathbf{x}) \log(p(\mathbf{x}) / q(\mathbf{x})) d\mathbf{X}$	Cmp, Det	#P-hard w/o Det
RÉNYI'S ALPHA DIV.	$(1 - \alpha)^{-1} \log \int p^\alpha(\mathbf{x}) q^{1-\alpha}(\mathbf{x}) d\mathbf{X}, \alpha \in \mathbb{N}$	Cmp, q Det	#P-hard w/o Det
	$(1 - \alpha)^{-1} \log \int p^\alpha(\mathbf{x}) q^{1-\alpha}(\mathbf{x}) d\mathbf{X}, \alpha \in \mathbb{R}$	Cmp, Det	#P-hard w/o Det
ITAKURA-SAITO DIV.	$\int [p(\mathbf{x}) / q(\mathbf{x}) - \log(p(\mathbf{x}) / q(\mathbf{x})) - 1] d\mathbf{X}$	Cmp, Det	#P-hard w/o Det
CAUCHY-SCHWARZ DIV.	$-\log \frac{\int p(\mathbf{x}) q(\mathbf{x}) d\mathbf{X}}{\sqrt{\int p^2(\mathbf{x}) d\mathbf{X} \int q^2(\mathbf{x}) d\mathbf{X}}}$	Cmp	#P-hard w/o Cmp
SQUARED LOSS	$\int (p(\mathbf{x}) - q(\mathbf{x}))^2 d\mathbf{X}$	Cmp	#P-hard w/o Cmp

compositionally derive the tractability of many more queries

	Query	Tract. Conditions	Hardness
CROSS ENTROPY	$-\int p(\mathbf{x}) \log q(\mathbf{x}) d\mathbf{X}$	Cmp, q Det	#P-hard w/o Det
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ITAKURA-SAITO DIV.	$\int [p(\mathbf{x}) / q(\mathbf{x}) - \log(p(\mathbf{x}) / q(\mathbf{x})) - 1] d\mathbf{X}$	Cmp, Det	#P-hard w/o Det
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SQUARED LOSS	$\int (p(\mathbf{x}) - q(\mathbf{x}))^2 d\mathbf{X}$	Cmp	#P-hard w/o Cmp

and prove hardness when some input properties are not satisfied

Composable tractable sub-routines

```
function kld(p, q)
    r = quotient(p, q)
    s = log(r)
    t = product(p, s)
    return integrate(t)
end
```

```
function ent(p)
    q = log(p)
    r = product(p, q)
    return -integrate(s)
end
```

```
function xent(p, q)
    r = log(q)
    s = product(p, r)
    return -integrate(s)
end
```

```
function alphadiv(p, q, alpha=1.5)
    r = real_pow(p, alpha)
    s = real_pow(q, 1.0-alpha)
    t = product(r, s)
    return log(integrate(t)) / (1.0-alpha)
end
```

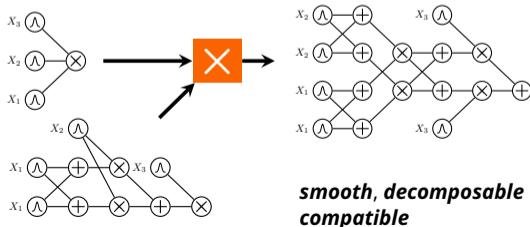
*Efficient inference algorithms in a couple lines of Julia code!*²

²<https://github.com/UCLA-StarAI/circuit-ops-atlas>

Next up...

1. Learning and reasoning with symbolic constraints
2. Expected predictions: handling missing values, fairness
3. Exact inference of causal effects

\Rightarrow using tractable operators



Symbolic constraints

“How can neural nets reason and learn with symbolic constraints reliably and efficiently?”

When?



Ground Truth

e.g. predict shortest path in a map

When?



Ground Truth

given \mathbf{x} // e.g. a tile map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid

structured output prediction (SOP) tasks

When?



Ground Truth

given \mathbf{x} // e.g. a tile map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid
s.t. $\mathbf{y} \models \mathbf{K}$ // e.g., that form a valid path

structured output prediction (SOP) tasks

When?



Ground Truth

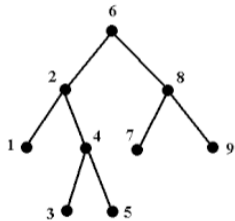
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find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. a configurations of edges in a grid
s.t. $\mathbf{y} \models \mathbf{K}$ // e.g., that form a valid path

// for a 12×12 grid, 2^{144} states but only 10^{10} valid ones!

structured output prediction (SOP) tasks

When?



given \mathbf{x} // e.g. a feature map

find $\mathbf{y}^* = \operatorname{argmax}_{\mathbf{y}} p_{\theta}(\mathbf{y} \mid \mathbf{x})$ // e.g. labels of classes

s.t. $\mathbf{y} \models \mathbf{K}$ // e.g., constraints over superclasses

$$\mathbf{K} : (Y_{\text{cat}} \implies Y_{\text{animal}}) \wedge (Y_{\text{dog}} \implies Y_{\text{animal}})$$

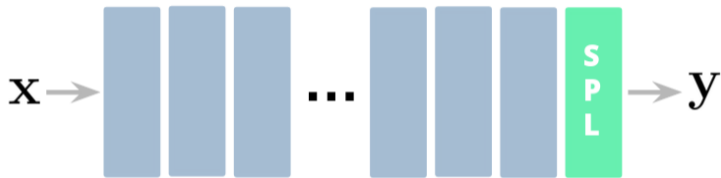
hierarchical multi-label classification

How?

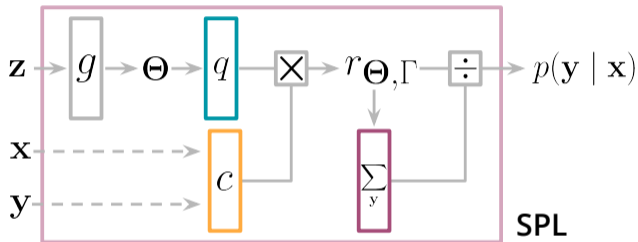


take an unreliable neural network architecture...

How?

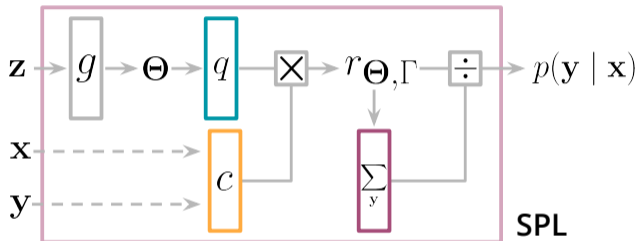


*.....and replace the last layer with
a semantic probabilistic layer*



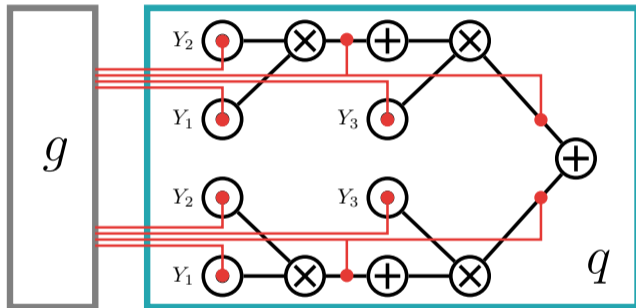
$q_{\Theta}(\mathbf{y} \mid g(\mathbf{z}))$ is an expressive distribution over labels

$c_{\mathbf{K}}(\mathbf{x}, \mathbf{y})$ encodes the constraint $\mathbb{1}\{\mathbf{x}, \mathbf{y} \models \mathbf{K}\}$

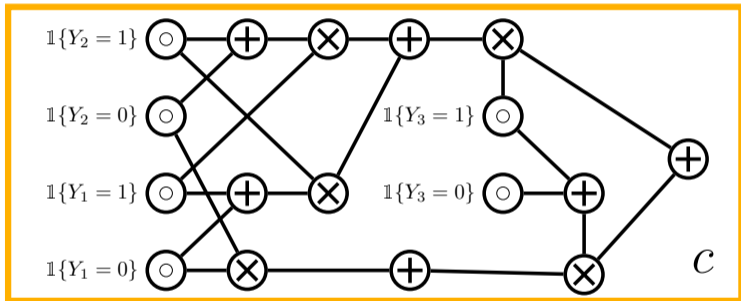


$$p(y | x) = q_{\Theta}(y | g(z)) \cdot c_K(x, y) / Z(x)$$

$$Z(x) = \sum_y q_{\Theta}(y | x) \cdot c_K(x, y)$$

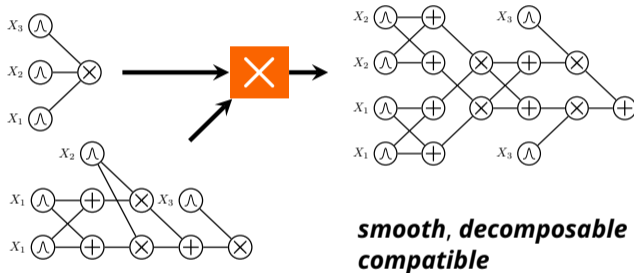


a conditional circuit $q(y; \Theta = g(z))$



and a logical circuit $c(y, x)$ encoding K

Tractable products



exactly compute \mathcal{Z} in time $O(|q||c|)$

SPL recipe

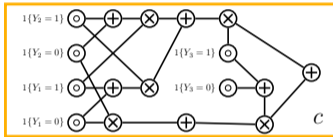
$$K : (Y_1 = 1 \implies Y_3 = 1)$$

$$\wedge (Y_2 = 1 \implies Y_3 = 1)$$

1) Take any
logical constraint

SPL recipe

$$K : (Y_1 = 1 \implies Y_3 = 1) \\ \wedge (Y_2 = 1 \implies Y_3 = 1)$$

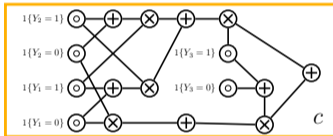


1) Take any
logical constraint

2) Compile it into
a constraint circuit

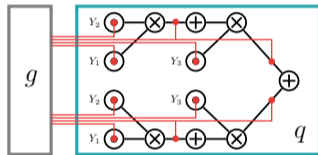
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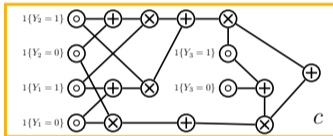
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3) Multiply it by a circuit distribution

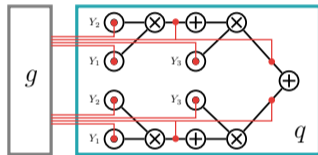
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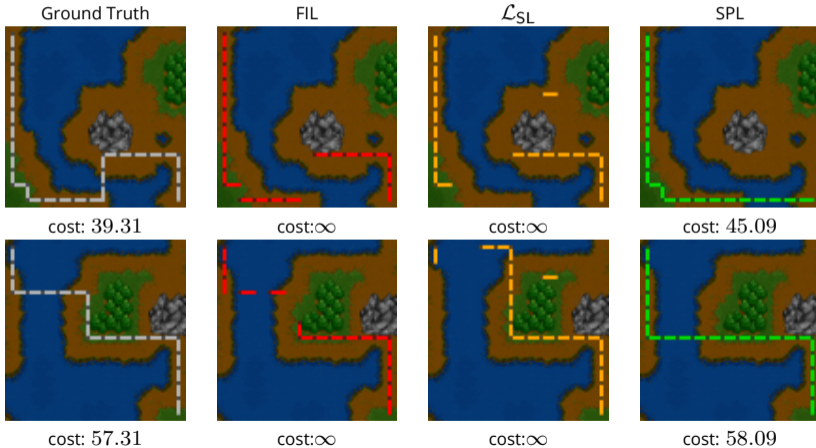
2) Compile it into a constraint circuit



3) Multiply it by a circuit distribution

4) train end-to-end by sgd!

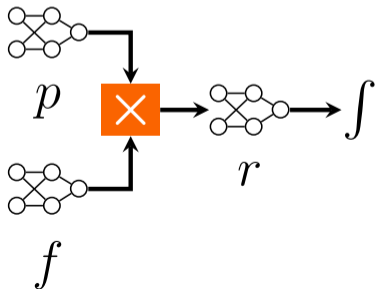
Guaranteeing consistency



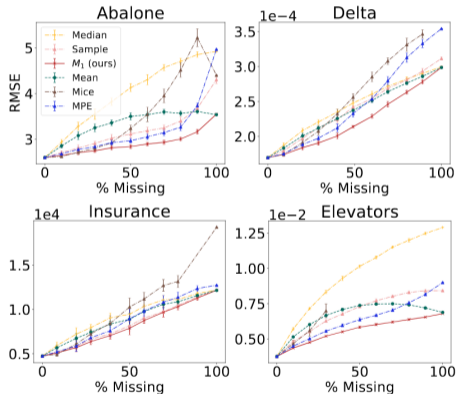
Expected predictions

Reasoning about the output of a classifier or regressor f given a distribution p over the input features

$$\mathbb{E}_p[f] = \int_{\text{val}(\mathbf{X})} p(\mathbf{x}) \times f(\mathbf{x}) d\mathbf{X}$$



Handling missing values at test time



Given a partial observation \mathbf{x}^o , what is the expected output from f ?

$$\mathbb{E}_{\mathbf{x}^m \sim p(\mathbf{x}^m | \mathbf{x}^o)} [f(\mathbf{x}^m, \mathbf{x}^o)]$$

Fairness analysis



```
using ProbabilisticCircuits
pc = load_prob_circuit(zoo_psdd_file("insurance.psdd"));
rc = load_logistic_circuit(zoo_lc_file("insurance.circuit"), 1);
```

q: *Is the predictive model biased by gender?*

```
groups = make_observations(["male"], ["female"])
exps, _ = Expectation(pc, rc, groups);
println("Female   : \$ $(exps[2])");
println("Male     : \$ $(exps[1])");
println("Diff      : \$ $(exps[2] - exps[1])");
Female   : $ 14170.125469335406
Male     : $ 13196.548926381849
Diff     : $ 973.5765429535568
```


Causal Inference

Given subsets $\mathbf{A}, \mathbf{Y} \subseteq \mathbf{X}$, interested in *causal effect* $p(\mathbf{Y}|\text{do}(\mathbf{A}))$.

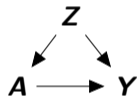
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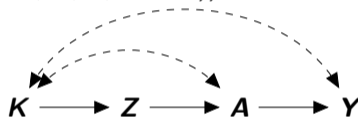
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- Specify (qualitative) assumptions on the system using a **causal diagram** G (here $\mathbf{A}, \mathbf{Y}, \mathbf{Z}, \mathbf{K} \subseteq \mathbf{X}$) :



(a) Backdoor

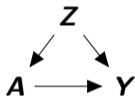


(b) Napkin

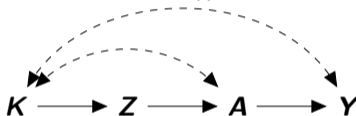
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(a) Backdoor



(b) Napkin

- Given causal diagram G , can derive expressions for causal effect $p(\mathbf{Y}|\mathbf{A})$ using *do-calculus* (Pearl 1995).

$$\sum_{\mathbf{Z}} p(\mathbf{Z})p(\mathbf{Y}|\mathbf{A}, \mathbf{Z})$$

(a) Backdoor

$$\frac{\sum_{\mathbf{K}} p(\mathbf{A}, \mathbf{Y}|\mathbf{K}, \mathbf{Z})p(\mathbf{K})}{\sum_{\mathbf{K}} p(\mathbf{A}|\mathbf{K}, \mathbf{Z})p(\mathbf{K})}$$

(b) Napkin

Tractability of Exact Causal Inference

Consider the backdoor query, for **fixed** values of the treatment \mathbf{a} and outcome \mathbf{y} :

$$p(\mathbf{y}|do(\mathbf{a})) := \sum_{\mathbf{Z}} p(\mathbf{Z}) \times p(\mathbf{y}|\mathbf{a}, \mathbf{Z})$$

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Theorem (Wang & Kwiatkowska 2023)

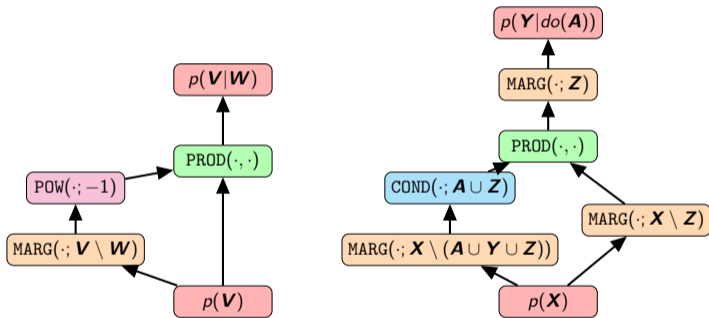
If p is given as a structured decomposable and deterministic circuit, then the backdoor query is #P-hard to compute.

Applying the Atlas of Tractable Operations

Break down do-calculus query into compositions of basic operations, such as marginalization, products, and powers:

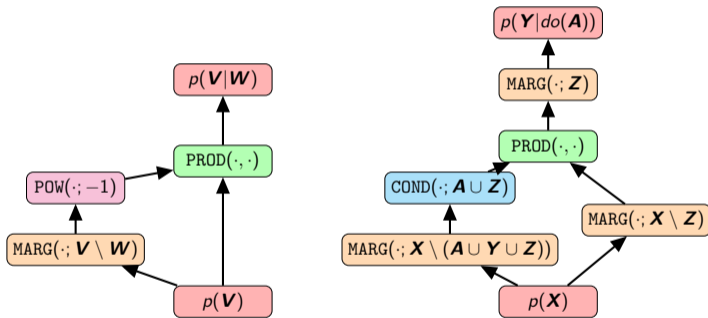
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Applying the Atlas of Tractable Operations

Break down do-calculus query into compositions of basic operations, such as marginalization, products, and powers:



(a) Pipeline for $\text{COND}(\cdot, \mathbf{W})$

(b) Pipeline for entire backdoor query

Problem: Cannot guarantee that input to POW is deterministic, even if $p(\mathbf{X})$ is deterministic.

Marginal Determinism

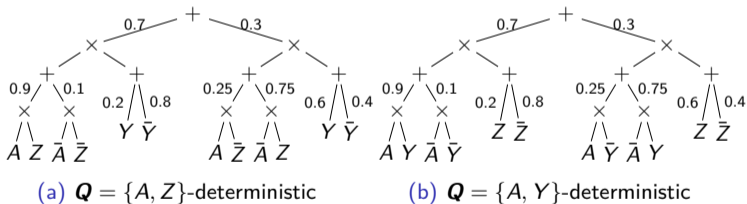
Definition (Marginal Determinism, Choi et al. 2020)

Given a subset of variables $Q \subseteq X$, a PC is Q -deterministic if the children of a sum node T correspond to different values of Q (for sum nodes with $sc(T) \cap Q \neq \emptyset$).

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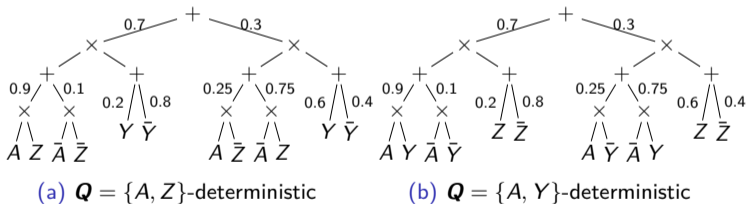
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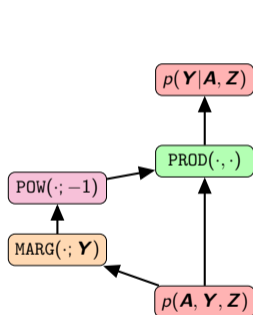
Motivation: If a circuit is marginally deterministic w.r.t Q , then we can marginalize out $X \setminus Q$ and obtain a deterministic circuit!

Tractable Causal Inference

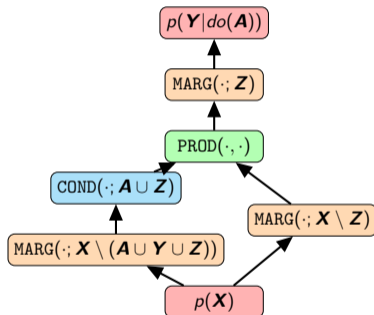
If (the circuit encoding) $p(\mathbf{X})$ is $(\mathbf{A} \cup \mathbf{Z})$ -deterministic, then the input to POW is guaranteed to be deterministic.

Tractable Causal Inference

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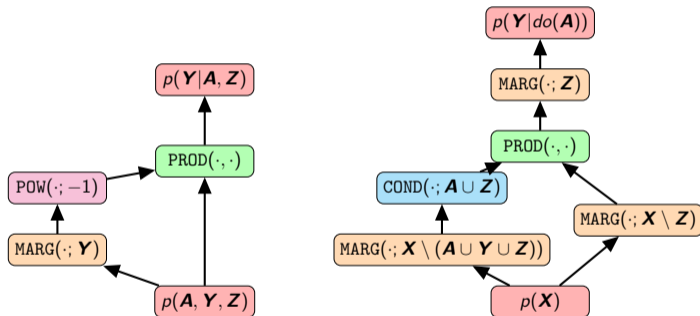
(a) Pipeline for $\text{COND}(\cdot, \mathbf{A} \cup \mathbf{Z})$



(b) Pipeline for entire backdoor query

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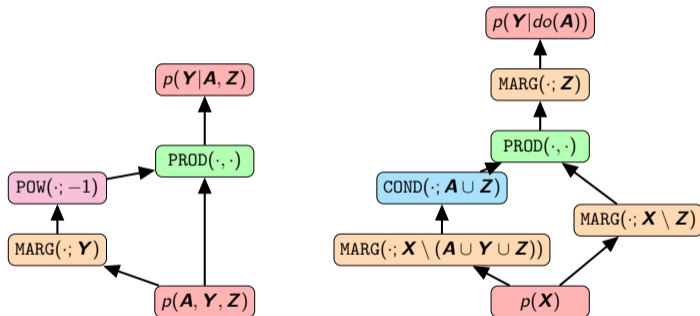
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(b) Pipeline for entire backdoor query

\implies all operations are tractable according to Atlas

Tractable Causal Inference

If (the circuit encoding) $p(\mathbf{X})$ is $(\mathbf{A} \cup \mathbf{Z})$ -deterministic, then the input to POW is guaranteed to be deterministic.



(a) Pipeline for $\text{COND}(\cdot, \mathbf{A} \cup \mathbf{Z})$

(b) Pipeline for entire backdoor query

\implies all operations are tractable according to Atlas

\implies can compute causal effect in $O(|p|^3)$ time

(can improve to $O(|p|^2)$)

Open Questions

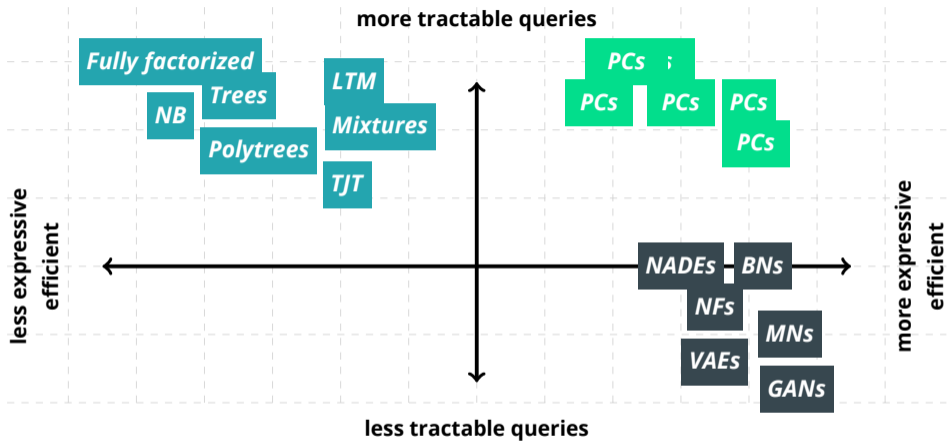
- ▶ Are all causal queries derived by the do-calculus tractable in PTIME (for some non-trivial marginal determinism condition)?
- ▶ What is the optimal complexity for these queries?

Questions answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
3. *What is the connection to logical circuit languages?* (YooJung)
4. *How do I compile my favorite model into a circuit?* (YooJung)
5. *How are circuit size and tractability related?* (YooJung)
6. *What's the most impressive query we can efficiently compute?* (YooJung)
7. *Are all tractable distributions probabilistic circuits?* (Guy)
8. *How to learn probabilistic circuits from data?* (Guy)

Questions answered today

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7. ***Are all tractable distributions probabilistic circuits?*** (Guy)
8. *How to learn probabilistic circuits from data?* (Guy)



tractability vs expressive efficiency

Smooth ∨ **decomposable** ∨ **deterministic**
 ∨ **structured decomposable** **PCs?**

	<i>smooth</i>	<i>dec.</i>	<i>det.</i>	<i>str.dec.</i>
Arithmetic Circuits (ACs) <i>(Darwiche 2003)</i>	✓	✓	✓	✗
Sum-Product Networks (SPNs) <i>(Poon et al. 2011)</i>	✓	✓	✗	✗
Cutset Networks (CNets) <i>(Rahman et al. 2014)</i>	✓	✓	✓	✗
Probabilistic Decision Graphs <i>(Jaeger 2004)</i>	✓	✓	✓	✓
(Affine) ADDs <i>(Hoey et al. 1999; Sanner et al. 2005)</i>	✓	✓	✓	✓
AndOrGraphs <i>(Dechter et al. 2007)</i>	✓	✓	✓	✓
PSDDs <i>(Kisa et al. 2014)</i>	✓	✓	✓	✓

Low-treewidth PGMs

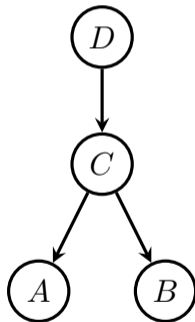
Tree, polytrees and
Thin Junction trees
can be turned into

- decomposable
- smooth
- deterministic

circuits

Therefore they support
tractable

- EVI
- MAR/CON
- MAP



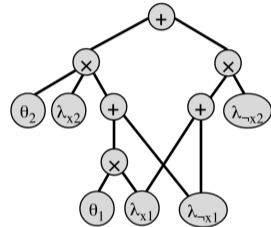
Arithmetic Circuits (ACs)

ACs (*Darwiche 2003*) are

- decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP



\Rightarrow parameters are attached to the leaves
 \Rightarrow ...but can be moved to the sum node edges (*Rooshenas et al. 2014*)

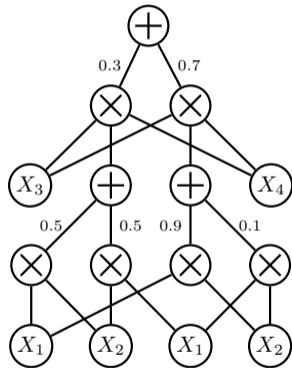
Sum-Product Networks (SPNs)

SPNs (Poon et al. 2011) are

- decomposable
- smooth
- ~~deterministic~~

They support tractable

- EVI
- MAR/CON
- ~~MAP~~



⇒ deterministic SPNs are also called selective (Peharz et al. 2014)

Cutset Networks (C Nets)

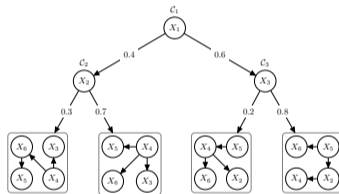
C Nets

(*Rahman et al. 2014*) are

- decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP



Rahman et al., "Cutset Networks: A Simple, Tractable, and Scalable Approach for Improving the Accuracy of Chow-Liu Trees", 2014

Di Mauro et al., "Learning Accurate Cutset Networks by Exploiting Decomposability", 2015

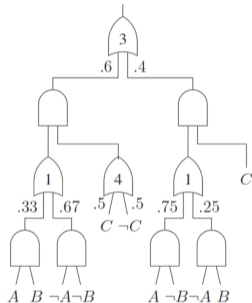
Probabilistic Sentential Decision Diagrams

PSDDs (Kisa et al. 2014) are

- structured decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP
- Complex queries!



Kisa et al., "Probabilistic sentential decision diagrams", 2014

Choi et al., "Tractable learning for structured probability spaces: A case study in learning preference distributions", 2015

Shen et al., "Conditional PSDDs: Modeling and learning with modular knowledge", 2018

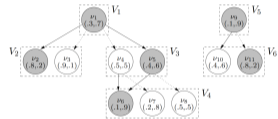
Probabilistic Decision Graphs

PDGs (Jaeger 2004) are

- structured
- decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP
- Complex queries!



Jaeger, "Probabilistic decision graphs—combining verification and AI techniques for probabilistic inference", 2004

Jaeger et al., "Learning probabilistic decision graphs", 2006

AndOrGraphs

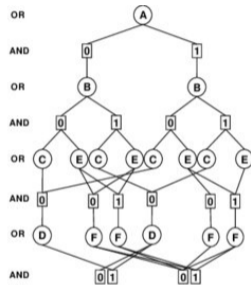
AndOrGarphs

(Dechter et al. 2007) are

- structured decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP
- Complex queries!



Dechter and Mateescu, "AND/OR search spaces for graphical models", 2007

Marinescu and Dechter, "Best-first AND/OR search for 0/1 integer programming", 2007

Probabilistic circuits seem awfully general.

*Are all tractable probabilistic models
probabilistic circuits?*



Enter: Determinantal Point Processes (DPPs)

DPPs are models where probabilities are specified by (sub)determinants

$$L = \begin{bmatrix} 1 & 0.9 & 0.8 & 0 \\ 0.9 & 0.97 & 0.96 & 0 \\ 0.8 & 0.96 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\Pr_L(X_1 = 1, X_2 = 0, X_3 = 1, X_4 = 0) = \frac{1}{\det(L + I)} \det(L_{\{1,2\}})$$

Enter: Determinantal Point Processes (DPPs)

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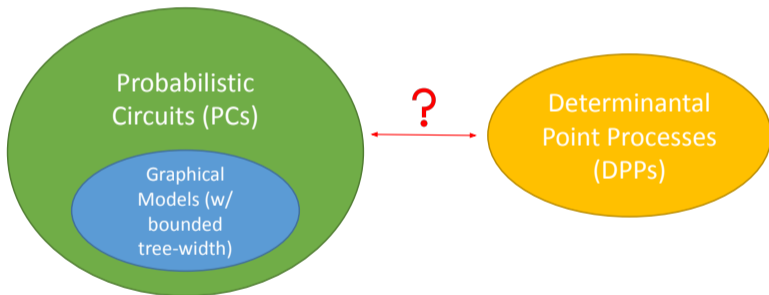
Tractable likelihoods and marginals

Global Negative Dependence

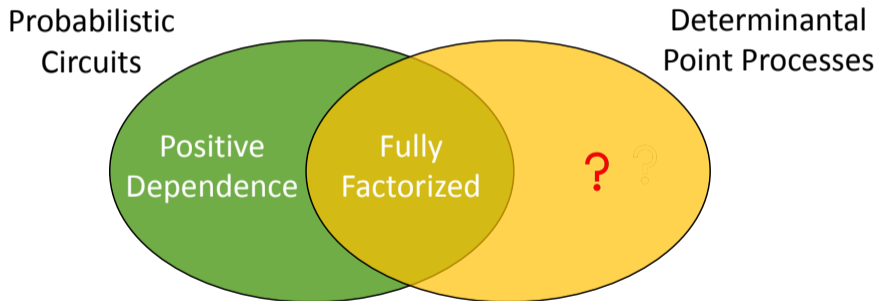
Diversity in recommendation systems

$$\Pr_L(X_1 = 1, X_2 = 0, X_3 = 1, X_4 = 0) = \frac{1}{\det(L + I)} \det(L_{\{1,2\}})$$

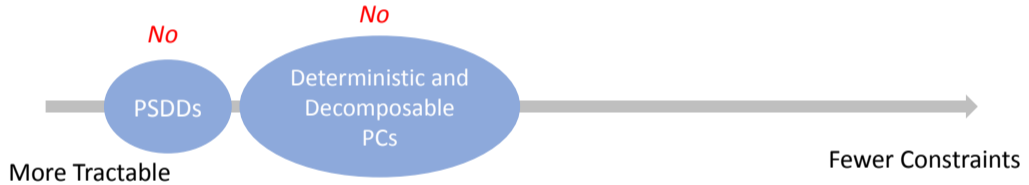
Are all tractable probabilistic models probabilistic circuits?



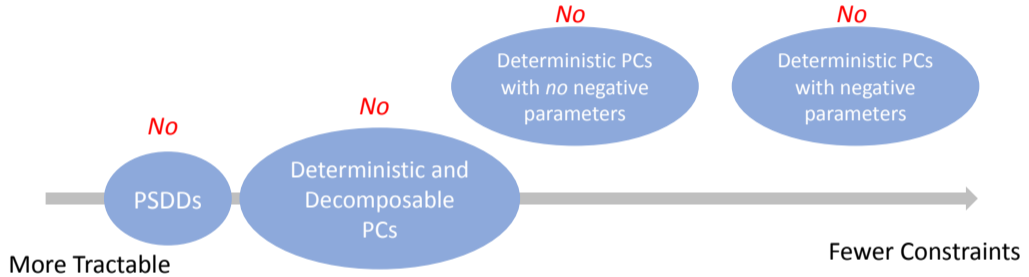
Relationship between PCs and DPPs



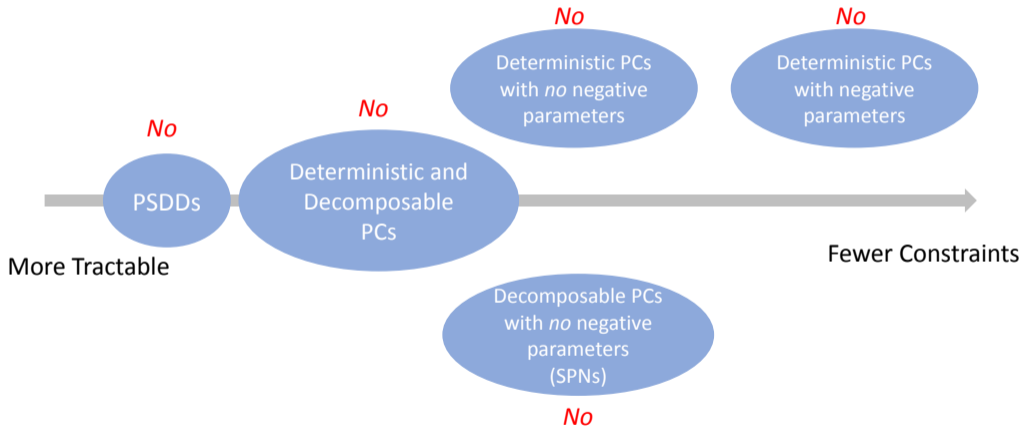
We cannot tractably represent DPPs with subclasses of PCs



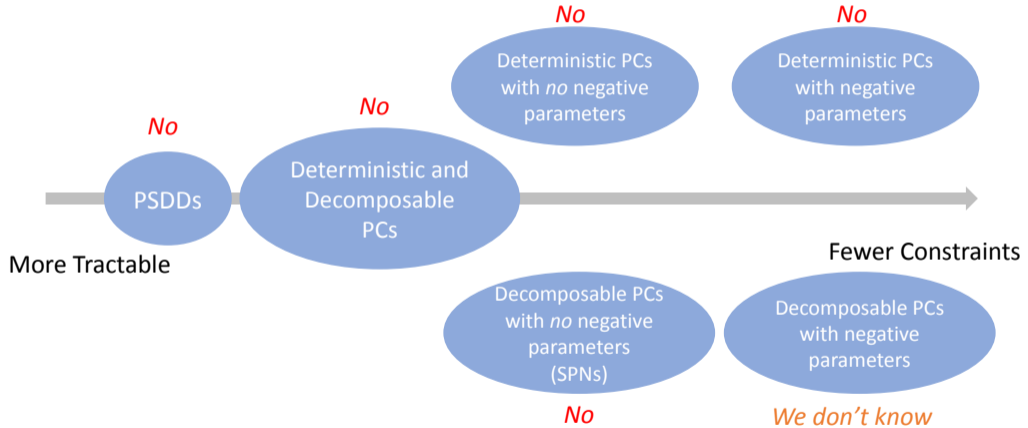
We cannot tractably represent DPPs with subclasses of PCs



We cannot tractably represent DPPs with subclasses of PCs



We cannot tractably represent DPPs with subclasses of PCs



PCs and Circuit Lower Bounds

Theorem (Martens and Medabalimi, 2014). *Let P_n be the uniform distribution over spanning trees on K_n . For $n \geq 20$, the size of any smooth and decomposable PC that represents P_n is at least $2^{n/30240}$.*

Based on arithmetic circuit lower bounds by Ran Raz and Amir Yehudayoff

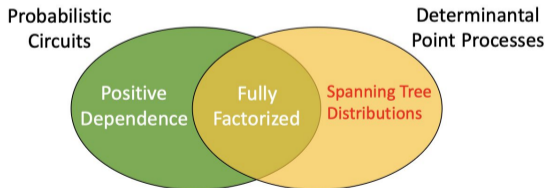
Decomposable PCs are Syntactically Multilinear Arithmetic Circuits:

Definition 7 (Multilinear Arithmetic Circuit) If every node of an arithmetic circuit Φ over y computes a multilinear polynomial in y , Φ is said to be a *(semantically) multilinear arithmetic circuit*. And if for every product node in Φ , the scopes of its child nodes are pair-wise disjoint, Φ is said to be a *syntactically multilinear arithmetic circuit*.

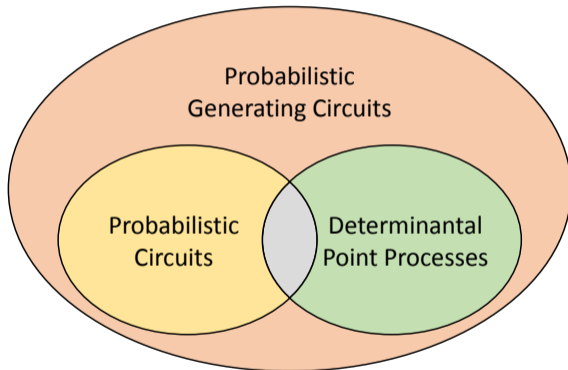
DPPs have No Compact Decomposable PCs

Theorem (Snell, 1995). *The uniform distribution over spanning trees on the complete graph K_n is a DPP over $\binom{n}{2}$ edges.*

Theorem (Martens and Medabalimi, 2014). *Let P_n be the uniform distribution over spanning trees on K_n . For $n \geq 20$, the size of any smooth and decomposable PC that represents P_n is at least $2^{n/30240}$.*



Probabilistic Generating Circuits



A Tractable Unifying Framework for PCs and DPPs

Probability Generating Functions

X_1	X_2	X_3	\Pr_β
0	0	0	0.02
0	0	1	0.08
0	1	0	0.12
0	1	1	0.48
1	0	0	0.02
1	0	1	0.08
1	1	0	0.04
1	1	1	0.16



$$g_\beta = 0.16z_1z_2z_3 + 0.04z_1z_2 + 0.08z_1z_3 + 0.02z_1 + 0.48z_2z_3 + 0.12z_2 + 0.08z_3 + 0.02.$$

Probability Generating Functions

X_1	X_2	X_3	\Pr_β
0	0	0	0.02
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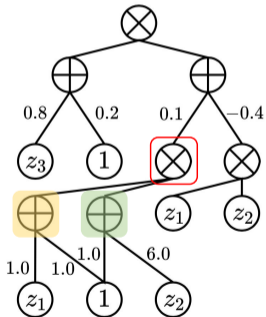
$$g_\beta = 0.16z_1z_2z_3 + 0.04z_1z_2 + 0.08z_1z_3 + 0.02z_1 \\ + 0.48z_2z_3 + 0.12z_2 + 0.08z_3 + 0.02.$$



$$g_\beta = (0.1(z_1 + 1))(6z_2 + 1) - 0.4z_1z_2)(0.8z_3 + 0.2)$$

Probabilistic Generating Circuits (PGCs)

$$g_{\beta} = (0.1(z_1 + 1)(6z_2 + 1) - 0.4z_1z_2)(0.8z_3 + 0.2)$$



1. Sum nodes \oplus with weighted edges to children.
2. Product nodes \otimes with unweighted edges to children.
3. Leaf nodes: z_i or constant.

PCs as PGCs

(Smooth & Decomposable) PCs represents probability mass functions:

$$m_{\beta} = 0.16X_1X_2X_3 + 0.04X_1X_2\bar{X}_3 + 0.08X_1\bar{X}_2X_3 + 0.02X_1\bar{X}_2\bar{X}_3 \\ + 0.48\bar{X}_1X_2X_3 + 0.12\bar{X}_1X_2\bar{X}_3 + 0.08\bar{X}_1\bar{X}_2X_3 + 0.02\bar{X}_1\bar{X}_2\bar{X}_3$$

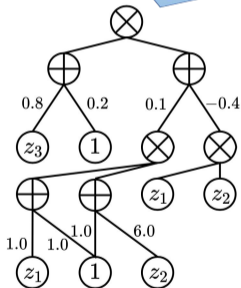
PGCs represent probability generating functions:

$$g_{\beta} = 0.16z_1z_2z_3 + 0.04z_1z_2 + 0.08z_1z_3 + 0.02z_1 \\ + 0.48z_2z_3 + 0.12z_2 + 0.08z_1z_3 + 0.02$$

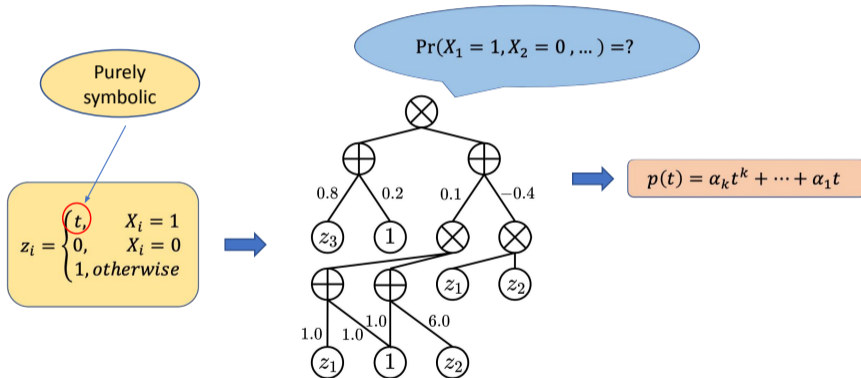
Given a smooth & decomposable PC, by setting \bar{X}_i to 1, and X_i to z_i , we obtain a PGC that represents the PC.

Tractable Likelihood (EVID) or Marginals (MAR)?

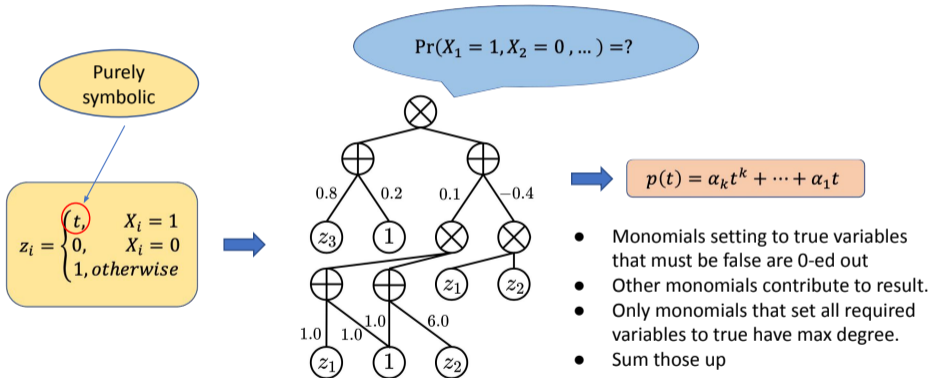
$$\Pr(X_1 = 1, X_2 = 0, \dots) = ?$$



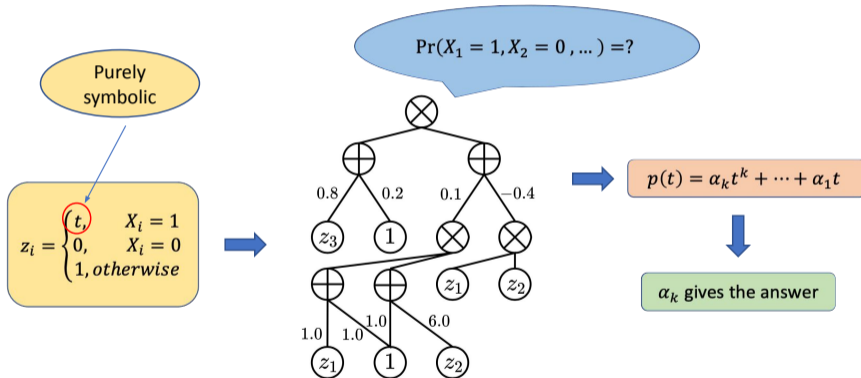
PGCs Support Tractable Likelihoods/Marginals



PGCs Support Tractable Likelihoods/Marginals

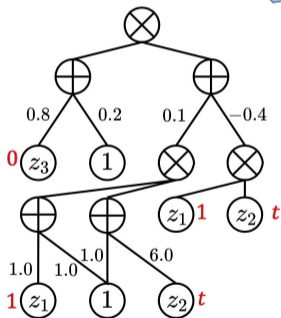


PGCs Support Tractable Likelihoods/Marginals

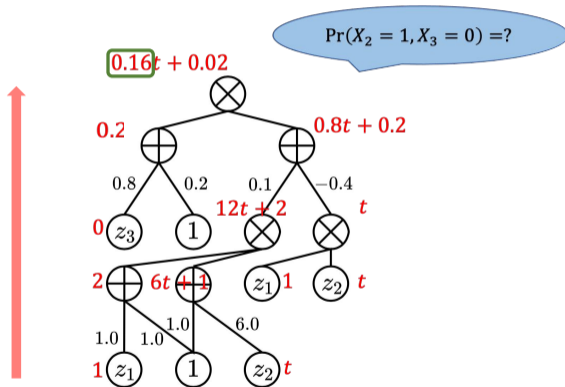


Example

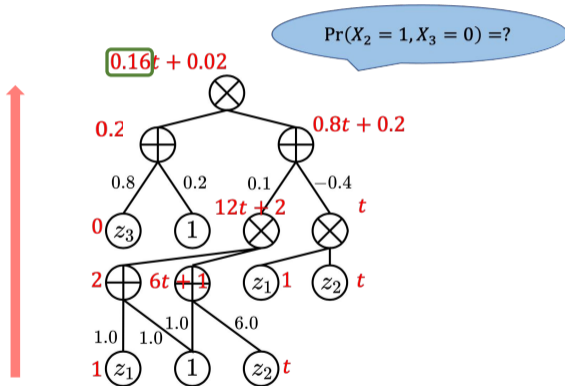
$$\Pr(X_2 = 1, X_3 = 0) = ?$$



Example



Example



X_1	X_2	X_3	\Pr_β
0	0	0	0.02
0	0	1	0.08
0	1	0	0.12
0	1	1	0.48
1	0	0	0.02
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1	1	1	0.16

Inference Time Complexity

Given a PGC of size m (#edges) over n random variables.

Algorithm 1 (Zhang *et al.*, ICML 2021):

$$\begin{array}{l} \text{Bottom-up pass} \\ \text{w/ } z_i = t, 0 \text{ or } 1 \end{array} + \begin{array}{l} \text{Product/sum of degree-}n \\ \text{polynomials at each node} \end{array} = \begin{array}{l} O(mn^2) \\ \text{or } O(mn \log n \log \log n) \end{array}$$

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Algorithm 2 (Harviainen et al., UAI 2023):

observation: the output of a PGC is a degree- n polynomial w/ respect to t

$$\begin{array}{l} \text{Bottom-up pass} \\ \text{w/ } t = 0, 1, \dots, n \end{array} + \begin{array}{l} \text{Polynomial interpolation at} \\ t = 0, 1, \dots, n \end{array} = \begin{array}{l} O(mn) \end{array}$$

Syntactic vs. Semantic Restrictions

- + PGCs are tractable when semantically multilinear
 - + No need for PC decomposability/syntactic multilinearity or other properties...
- Checking Validity of PGCs is Hard

Theorem (*Harviainen et al.*). It is NP-hard to check if a PGC encodes a valid probability generating polynomial

DPPs as PGCs

The generating polynomial for a DPP with kernel L is given by:

$$g_L = \frac{1}{\det(L + I)} \det(I + L \text{diag}(z_1, \dots, z_n)).$$

We need it as a sum of products to obtain a
Probabilistic Generating Circuit

DPPs as PGCs

The generating polynomial for a DPP with kernel L is given by:

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Constant



We need it as a sum of products to obtain a Probabilistic Generating Circuit

DPPs as PGCs

The generating polynomial for a DPP with kernel L is given by:

$$g_L = \frac{1}{\det(L + I)} \det(I + L \text{diag}(z_1, \dots, z_n)).$$

Constant

Division-free determinant algorithm
(Samuelson-Berkowitz algorithm)

g_L can be represented as a PGC of size $O(n^4)$

Experiment Results: Amazon Baby Registries

	DPP	Strudel	EiNet	MT	SimplePGC
apparel	-9.88	-9.51	-9.24	-9.31	-9.10 ^{*†°}
bath	-8.55	-8.38	-8.49	-8.53	-8.29 ^{*†°}
bedding	-8.65	-8.50	-8.55	-8.59	-8.41 ^{*†°}
carseats	-4.74	-4.79	-4.72	-4.76	-4.64 ^{*†°}
diaper	-10.61	-9.90	-9.86	-9.93	-9.72 ^{*†°}
feeding	-11.86	-11.42	-11.27	-11.30	-11.17 ^{*†°}
furniture	-4.38	-4.39	-4.38	-4.43	-4.34 ^{*†°}
gear	-9.14	-9.15	-9.18	-9.23	-9.04 ^{*†°}
gifts	-3.51	-3.39	-3.42	-3.48	-3.47 [°]
health	-7.40	-7.37	-7.47	-7.49	-7.24 ^{*†°}
media	-8.36	-7.62	-7.82	-7.93	-7.69 ^{†°}
moms	-3.55	-3.52	-3.48	-3.54	-3.53 [°]
safety	-4.28	-4.43	-4.39	-4.36	-4.28 ^{*†°}
strollers	-5.30	-5.07	-5.07	-5.14	-5.00 ^{*†°}
toys	-8.05	-7.61	-7.84	-7.88	-7.62 ^{†°}

SimplePGC achieves SOTA
result on 11/15 datasets

Beyond DPPs: Strongly Rayleigh Distributions

DPPs are strongly Rayleigh distributions

Definition. *A probability distribution over binary random variables X_1, \dots, X_n (or equivalently, subsets of $[n] := \{1, 2, \dots, n\}$) is strongly Rayleigh if its probability generating polynomial g is real-stable; that is, for $z_i \in \mathbb{C}$, if $\text{Im}(z_i) > 0$ for all z_i , then $g(z_1, \dots, z_n) \neq 0$.*

We can efficiently sample from strongly Rayleigh distributions by MCMC (with polynomial bound on mixing time)

Efficient Sampling from SR Distributions

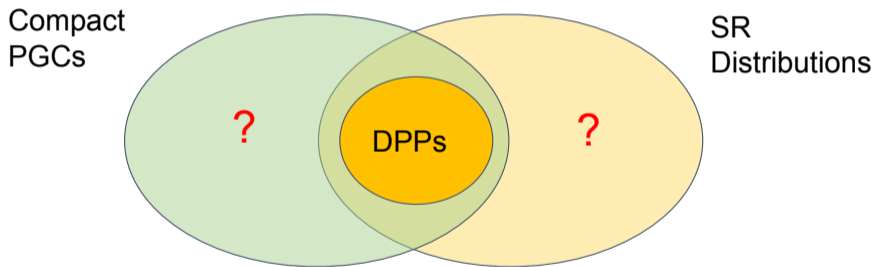
Theorem (Li et al., 2016). *Let π be a strongly Rayleigh distribution over $[n]$, we can efficiently sample from π by sampling from its symmetric homogenization π_{sh} ; for $S \subset [2n]$, define*

$$\pi_{sh}(S) := \begin{cases} \pi(S \cap [n]) \binom{n}{S \cap [n]}^{-1}, & \text{if } |S| = n \\ 0, & \text{otherwise} \end{cases}$$

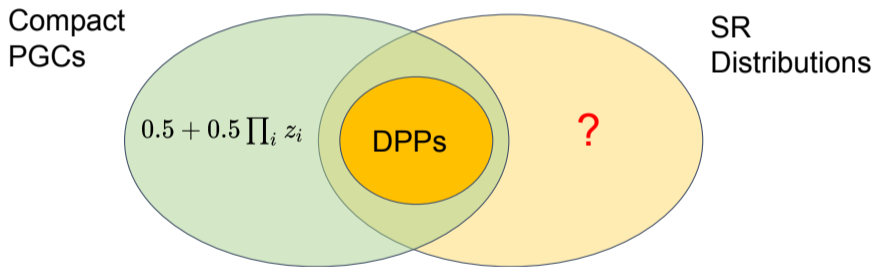
in particular, π_{sh} is also strongly Rayleigh and the mixing time of a Gibbs-exchange sampler with initial set S_0 is bounded as

$$\tau(\epsilon) \leq 2n^2 \left(\log \binom{n}{|S_0|} + \log \pi(S_0)^{-1} + \log \epsilon^{-1} \right)$$

Relationship between PGCs and SR Distributions



Relationship between PGCs and SR Distributions



Not All SR Distributions have Compact PGCs (Bläser 2023)

Let $K_{m,n} = (U \cup V, E)$ be a complete bipartite graph, the signed double function generating polynomial is defined as

$$DF_{m,n}(e) = \sum_{F,H} (-1)^{|F|+|H|} \prod_{(i,j) \in F} e_{i,j} \prod_{(i',j') \in H} e_{i',j'}$$

where the sum is taken over all partial functions $U \rightarrow V$ and $V \rightarrow U$, respectively. Each pair of (F, H) is a double function of $K_{m,n}$.

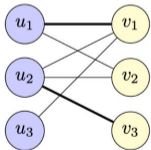


Figure 4. The thick edges are a matching of size two.

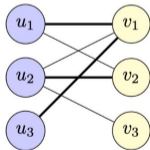


Figure 5. The thick edges form a total function $U \rightarrow V$, which is not injective.

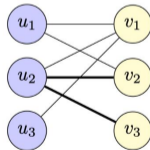


Figure 6. The thick edges form a partial function from V to U .

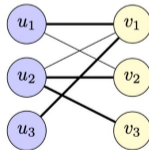



Figure 7. A double function.

Not All SR Distributions have Compact PGCs (Bläser 2023)

$$DF_{m,n}(e) = \sum_{F,H} (-1)^{|F|+|H|} \prod_{(i,j) \in F} e_{i,j} \prod_{(i',j') \in H} e_{i',j'}$$

 Generalize to bipartite multigraph $K_{m,n}^{(d)}$
 d : each edge from U to V has d copies

$$DF_{m,n}^{(d)}(e^{(d)}) = \sum_{F,H} (-1)^{|F|+|H|} \prod_{(i,j) \in F \setminus H} \sum_{\delta=1}^d e_{i,j}^{(\delta)} \prod_{(i',j') \in H \cap F} \sum_{1 \leq \delta' < \gamma \leq d} e_{i',j'}^{(\delta')} e_{i',j'}^{(\gamma)} \prod_{(i'',j'') \in H \setminus F} \sum_{\delta''=1}^d e_{i'',j''}^{(\delta'')}$$

$DF_{n,n}^{(n+2)}$ is real-stable and its evaluation is #P-hard.

$DF_{n,n}^{(n+2)}$ does not define an SR distribution as it has negative coefficients

Not All SR Distributions have Compact PGCs (Bläser 2023)

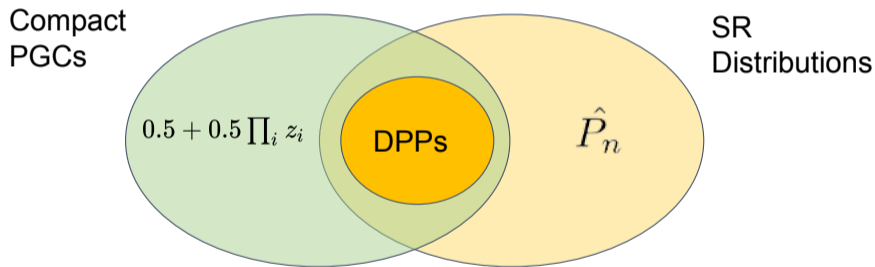
Definition. For a polynomial $f(z_1, \dots, z_n)$ with z_i of degree k_i , the inversion of f is defined as $\prod_i z_i^{k_i} f(-1/z_1, \dots, -1/z_i, \dots, -1/z_n)$.

The inversion of a real stable polynomial is also real stable

Let P_n be the inversion of $DF_{n,n}^{(n+2)}$, then P_n is a multilinear and real stable polynomial with all coefficients non-negative.

Theorem (Bläser, 2023). Assuming $P^{\#P} \not\subseteq P/\text{Poly}$. Let \hat{P}_n be the normalized P_n , then \hat{P}_n cannot be represented as polynomial-size PGCs.

Relationship between PGCs and SR Distributions



Probabilistic **generating** circuits seem awfully general.

*Are all tractable probabilistic models probabilistic **generating** circuits?*



Questions answered today

1. *What are probabilistic queries? Are current models tractable?* (Guy)
2. *What are probabilistic circuits and why are they tractable?* (Guy)
3. *What is the connection to logical circuit languages?* (YooJung)
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4. *How do I compile my favorite model into a circuit?* (YooJung)
5. *How are circuit size and tractability related?* (YooJung)
6. *What's the most impressive query we can efficiently compute?* (YooJung)
7. ***Are all tractable distributions probabilistic circuits?*** (Guy)
8. *How to learn probabilistic circuits from data?* (Guy)

Building Probabilistic Circuits

Information

Prior Knowledge

domain assumptions
constraints
other models

Data

experimental data
samples
measurements

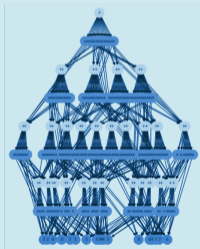
compilation



learning

Circuits

Structure



Parameters

θ, w

generative
discriminative
Bayesian
credal

decomposability
smoothness
determinism
compatibility

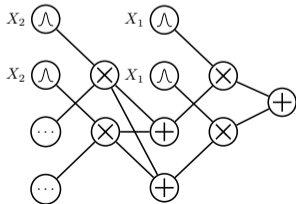
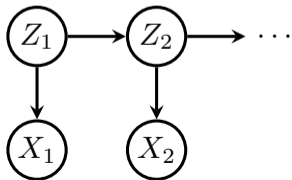
Origins: Compilation

Compiling probabilistic graphical models

Arithmetic circuits

(Darwiche 2002, 2003, 2009)

- Compile a given Bayesian network into an **arithmetic circuit**—a smooth, decomposable and deterministic PCs
- Either via logic encoding of Bayesian network + knowledge compilation
- Or record “execution trace” (sum and product operations) of traditional inference algorithms (junction tree, variable elimination)



Compilation

Selected references

Logic circuits, interplay between structural properties and tractable reasoning

(Darwiche et al. 2002a)

Converting probabilistic graphical models via knowledge compilation

(Darwiche 2002)

Logic circuit compilers

(Darwiche 2004; Muise et al. 2012; Bova et al. 2015; Lagniez et al. 2017; Oztok et al. 2018)

Neuro-symbolic models using logic circuits

(Ahmed et al. 2022a,b)

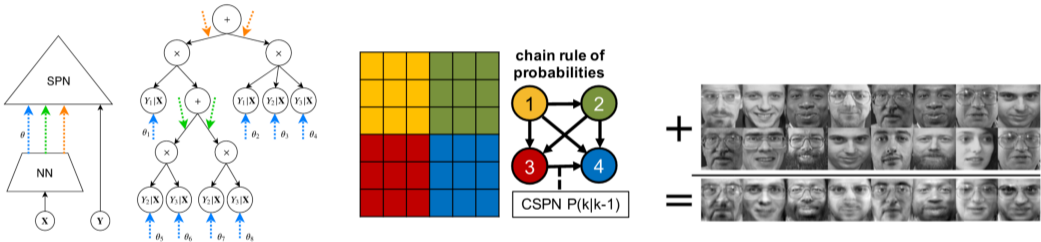
Parameter Learning

Gradient descent (of course)

- PCs are computational graphs
- Hence we can just learn them as any other neural net using SGD
- Use re-parameterization if parameters should satisfy constraints:
 - soft-max for sum-weights (non-negative, sum-to-one)
 - soft-plus for variances
 - low-rank plus diagonal for covariance matrices
- Allows for conditional distributions

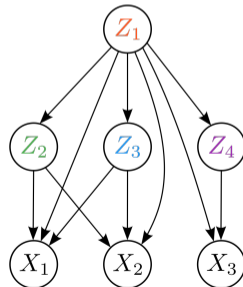
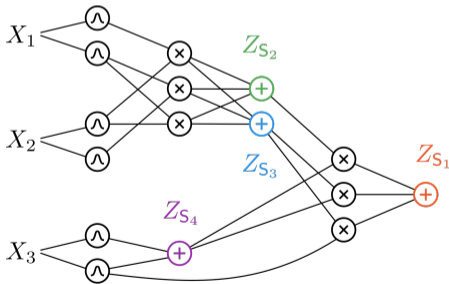
Conditional PCs

(Shao et al. 2019)



Maximum likelihood (frequentist)

PCs can be interpreted as **hierarchical latent variable models**, where each sum node corresponds to a discrete latent variable (*Peharz et al. 2016*). This allows to perform **classical maximum-likelihood** estimation.



Closed-form maximum likelihood

When the circuit is **deterministic**, there is even an **closed-form ML solution**, which is incredible fast:

```
julia> using ProbabilisticCircuits;
julia> data, structure = load(...);
julia> num_examples(data)
17412
julia> num_edges(structure)
270448
julia> @btime estimate_parameters(structure, data);
63.585 ms (1182350 allocations: 65.97 MiB)
```



Custom SIMD and CUDA kernels to parallelize over layers and training examples.

<https://github.com/Juice-jl/>

Expectation-Maximization

When the PC is not deterministic, we can still apply **expectation-maximization** (Peharz *et al.* 2016). EM can piggy-back on autodiff:

```
train_x, valid_x, test_x = get_mnist_images([7])

graph = Graph.poon_domingos_structure(shape=(28,28), delta=[7])
args = EinsumNetwork.Args(num_var=train_x.shape[1], num_dims=1,
                          num_classes=1, num_sums=28,
                          num_input_distributions=28,
                          exponential_family=EinsumNetwork.BinomialArray,
                          exponential_family_args={'N':255},
                          online_em_frequency=1, online_em_stepsize=0.05)

PC = EinsumNetwork.EinsumNetwork(graph, args)
PC.initialize()
PC.to('cuda')
```


Expectation-Maximization

```
for epoch_count in range(10):
    train_ll, valid_ll, test_ll = compute_loglikelihood()
    start_t = time.time()

    for idx in get_batches(train_x, 100):
        outputs = PC.forward(train_x[idx, :])
        log_likelihood = EinsumNetwork.log_likelihoods(outputs).sum()
        log_likelihood.backward()
        PC.em_process_batch()

    print_performance(epoch_count, train_ll, valid_ll, test_ll, time.time() - start_t)
```

Expectation-Maximization

```
# train sample: 5175  
# parameters: 1573486
```

```
[epoch 0]  train LL -140936.80   valid LL -140955.72   test LL -141033.80   ... elapsed time 3.621 sec  
[epoch 1]  train LL -15916.14    valid LL -15693.25   test LL -15976.43   ... elapsed time 3.438 sec  
[epoch 2]  train LL -10865.67    valid LL -10616.72   test LL -10943.56   ... elapsed time 3.436 sec  
[epoch 3]  train LL -10388.53    valid LL -10158.84   test LL -10475.49   ... elapsed time 3.473 sec  
[epoch 4]  train LL -10264.11    valid LL -10041.66   test LL -10352.59   ... elapsed time 3.497 sec  
[epoch 5]  train LL -10212.66    valid LL -10001.09   test LL -10319.35   ... elapsed time 3.584 sec  
[epoch 6]  train LL -10192.21    valid LL -9965.98    test LL -10314.84   ... elapsed time 3.508 sec  
[epoch 7]  train LL -10153.97    valid LL -9920.09    test LL -10261.41   ... elapsed time 3.446 sec  
[epoch 8]  train LL -10112.95    valid LL -9882.48    test LL -10236.34   ... elapsed time 3.579 sec  
[epoch 9]  train LL -10093.31    valid LL -9862.15    test LL -10200.94   ... elapsed time 3.483 sec
```

Structure Learning

Region graphs

Laying out the PC structure on a high level

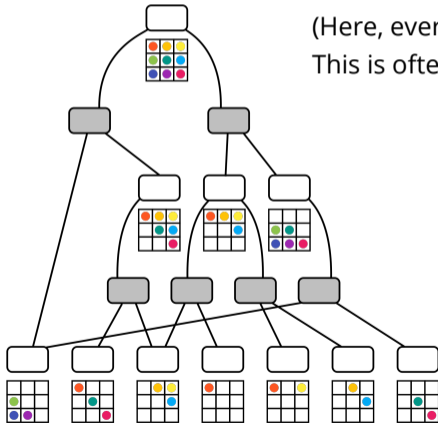
- Region graphs (RGs) describe decompositional structure
- RGs are *bipartite, directed graphs* containing *regions* (\mathcal{R}) and *partitions* (\mathcal{P})
- Input and output nodes of the RG are regions
- Regions have a *scope* (receptive field), denoted as $sc(\mathcal{R}) \subseteq \mathbf{X}$
- For every partition \mathcal{P} it holds that

$$sc(\mathcal{R}_{out}) = \bigcup_{\mathcal{R}_{in} \in inputs(\mathcal{P})} sc(\mathcal{R}_{in})$$

$$sc(\mathcal{R}') \cap sc(\mathcal{R}'') = \emptyset, \quad \mathcal{R}' \neq \mathcal{R}'' \in inputs(\mathcal{P})$$

Example region graph

X_1	X_2	X_3
X_4	X_5	X_6
X_7	X_8	X_9



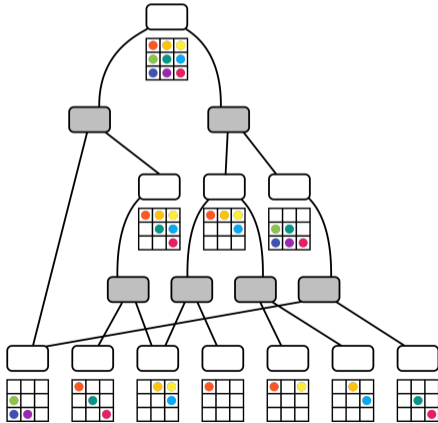
(Here, every partition has 2 input regions.
This is often assumed, but not necessary.)

From region graphs to PCs

X_1	X_2	X_3
X_4	X_5	X_6
X_7	X_8	X_9

\mathcal{R} 

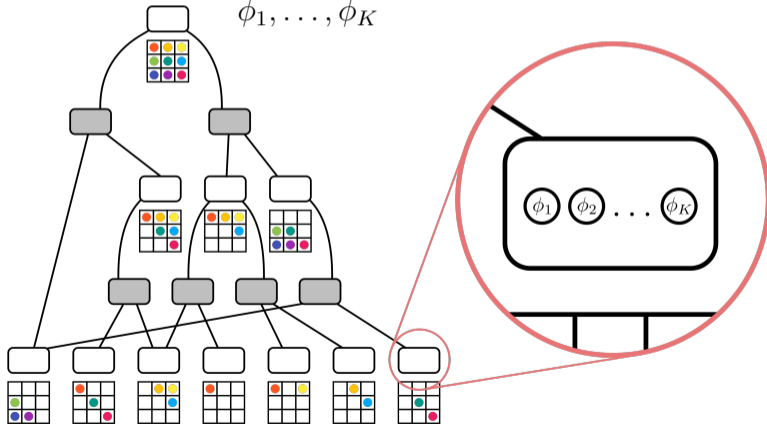
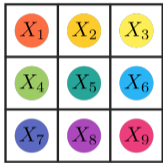
\mathcal{P} 



From region graphs to PCs

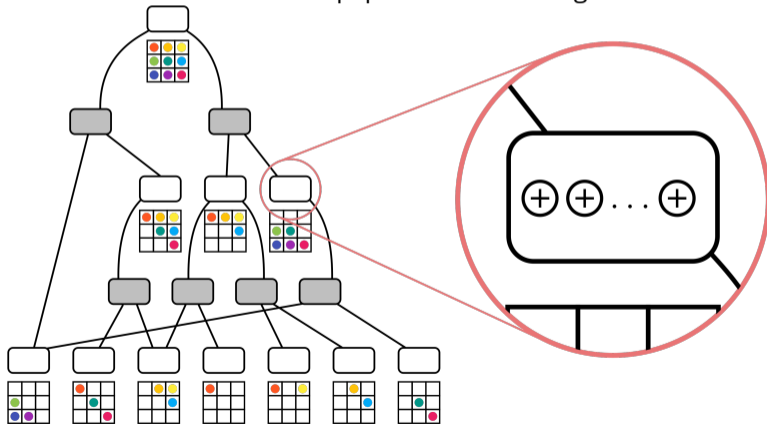
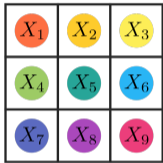
Equip each input region with non-linear units

ϕ_1, \dots, ϕ_K



From region graphs to PCs

Equip each internal region with sum nodes

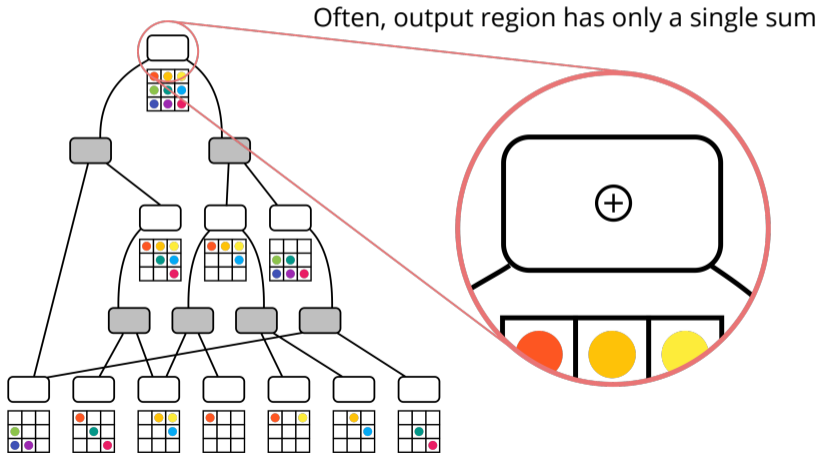


From region graphs to PCs

X_1	X_2	X_3
X_4	X_5	X_6
X_7	X_8	X_9

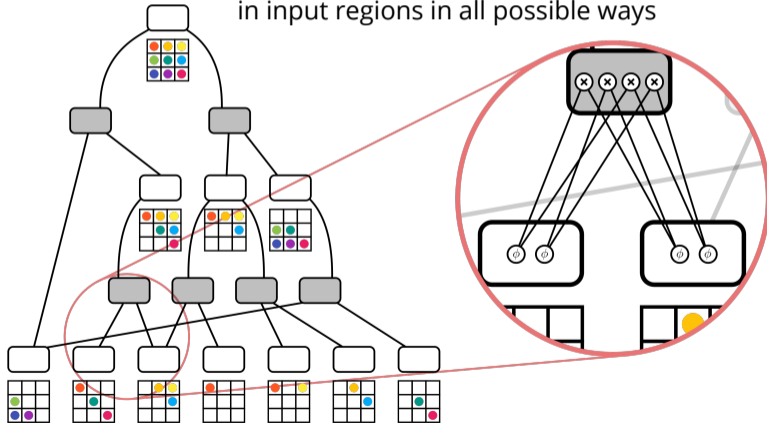
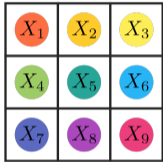
\mathcal{R} 

\mathcal{P} 



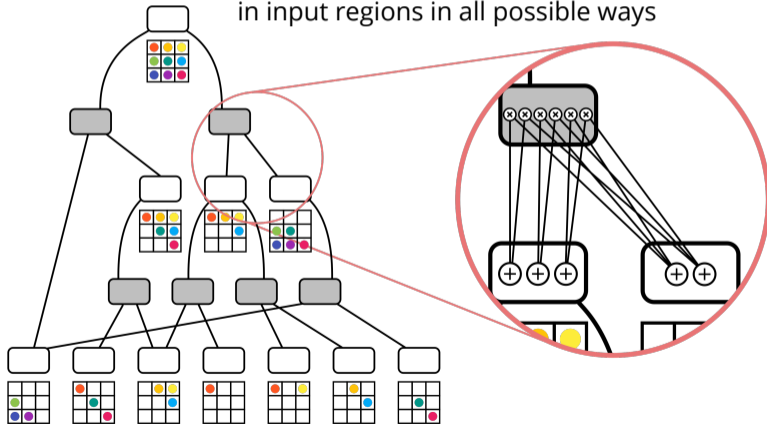
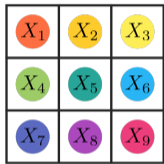
From region graphs to PCs

Equip partitions with products, combining units in input regions in all possible ways

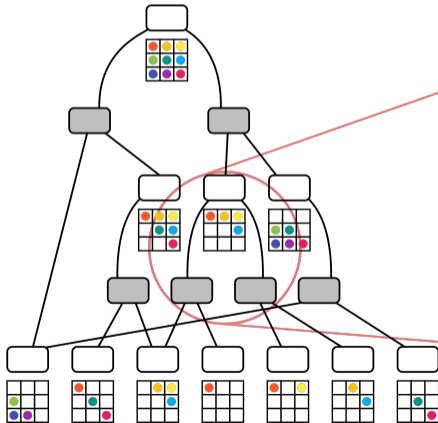
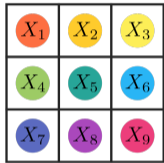


From region graphs to PCs

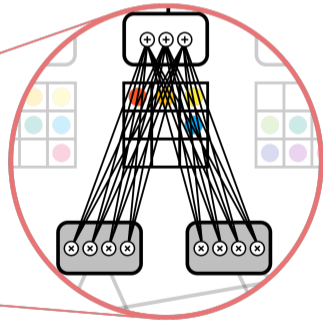
Equip partitions with products, combining units in input regions in all possible ways



From region graphs to PCs



Connect products to sum units above



From region graphs to PCs

- Equip each *input region* (leaf) \mathcal{R} with K units ϕ_1, \dots, ϕ_K , which are non-linear functions over $sc(\mathcal{R})$. Usually, ϕ_1, \dots, ϕ_K are probability densities. K can be different for each input region.
- Equip *each other region* with K sum units. K can be different for each internal region. Often, for the root region $K = 1$, when PC is used as density estimator.
- Equip each *partition* \mathcal{P} with as many products as there are combinations of units in the input regions to \mathcal{P} , selecting one unit from each region. Formally, if \mathcal{P} has input regions $\mathcal{R}_1, \mathcal{R}_2, \dots, \mathcal{R}_I$, insert one product $\prod_{i=1}^I u_i$ for each $(u_1, u_2, \dots, u_I) \in \mathcal{R}_1 \times \mathcal{R}_2 \times \dots \times \mathcal{R}_I$.
- Connect each $\prod_{i=1}^I u_i$ in \mathcal{P} to all sum units in the output regions of \mathcal{P} .

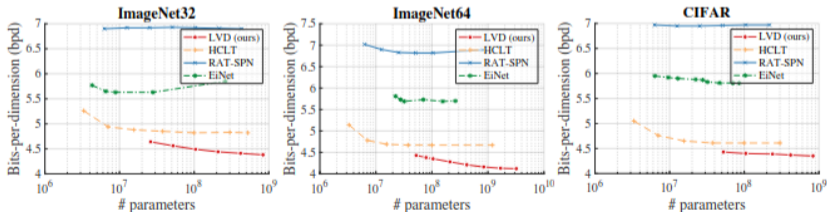
From region graphs to PCs

- Resulting PC has alternating sum and product units (not a strong constraint)
- We can easily scale the PC (overparameterize, increase expressivity) by equipping regions with more units
- RGs can be seen as a *vectorized version of PCs* – each region and partition can be seen as as a module
- Resulting PC will be *smooth and decomposable*, i.e., we can integrate, marginalize, and take conditionals
- After the PC has been constructed, we might discard the RG

Scaling up image models

Latent Variable Distillation

Dataset	TPMs				DGMs		
	LVD (ours)	HCLT	EiNet	RAT-SPN	Glow	RealNVP	BIVA
ImageNet32	4.38	4.82	5.63	6.90	4.09	4.28	3.96
ImageNet64	4.12	4.67	5.69	6.82	3.81	3.98	-
CIFAR	4.37	4.61	5.81	6.95	3.35	3.49	3.08



How to construct and learn RGs?

Random regions graphs

The “no-learning” option

(Peharz et al. 2019)

Generating a random region graph, by recursively splitting \mathbf{X} into two random parts:

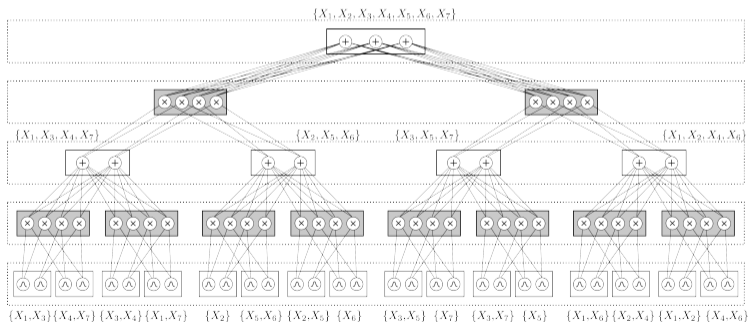


Image-tailored circuit structure

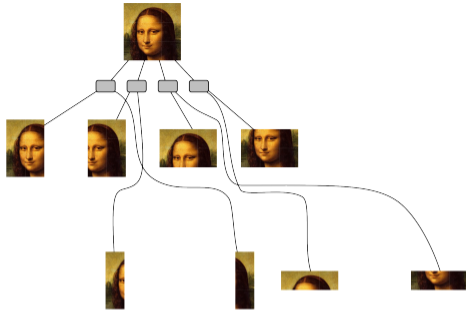
"Recursive image slicing"

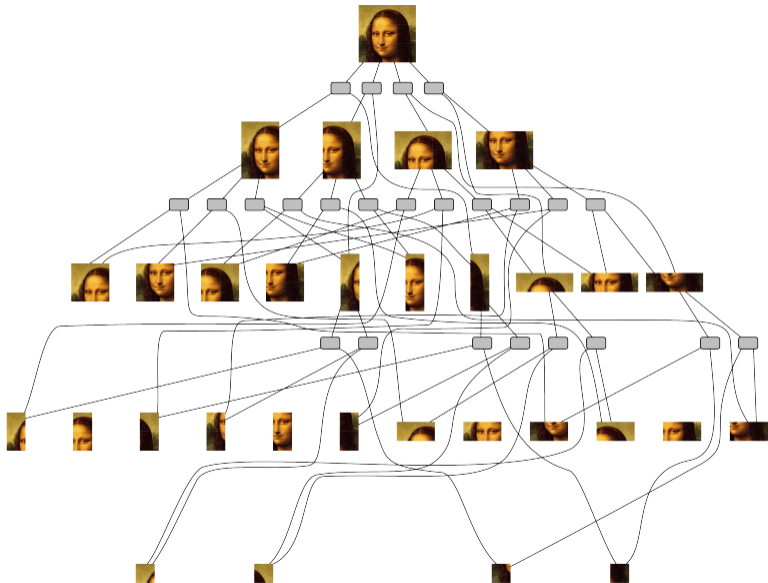
(Poon et al. 2011)

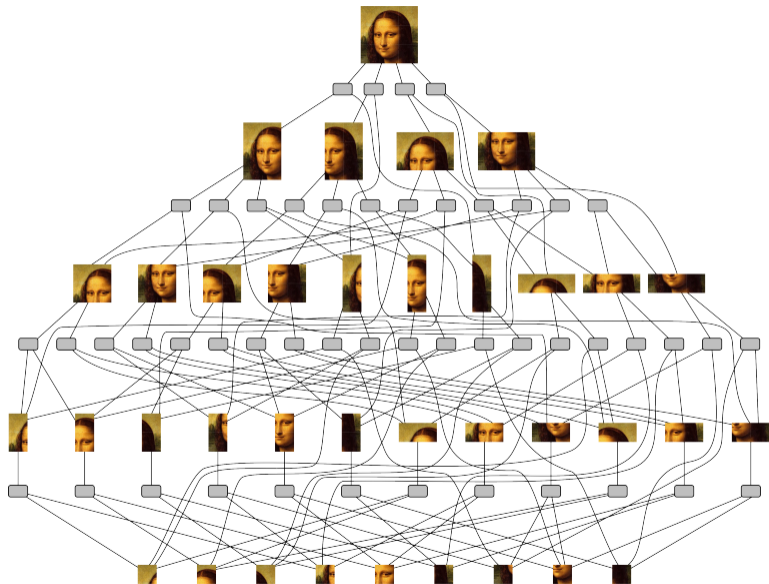
Images yield a natural region graph by using *axis-aligned splits*:

- Start with the full image (=output region)
- Define partitions by applying *horizontal* and *vertical* splits
- Recurse on the newly generated sub-images (internal regions)
- Structure somewhat reminiscent to convolutions
- Generates RGs which are "true DAGs," i.e. regions get re-used









Data-driven structure learning

"Recursive data slicing"

Expand regions with **clustering**

X_1	X_2	X_3	X_4	X_5

(Gens et al. 2013)



Data-driven structure learning

"Recursive data slicing"

Number of clusters = number of partitions



(Gens et al. 2013)

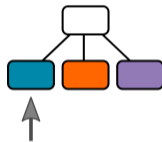
Data-driven structure learning

"Recursive data slicing"

Try to find independent groups of variables
(e.g. independence tests)



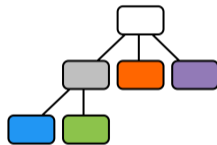
(Gens et al. 2013)



Data-driven structure learning

"Recursive data slicing"

Success → **partition** into new regions



(Gens et al. 2013)

Data-driven structure learning

"Recursive data slicing"

Try to find independent groups of variables
(e.g. independence tests)



(Gens et al. 2013)

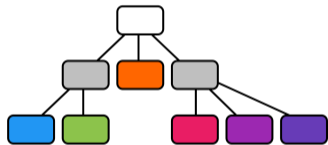
Data-driven structure learning

"Recursive data slicing"

Success → **partition** into new regions



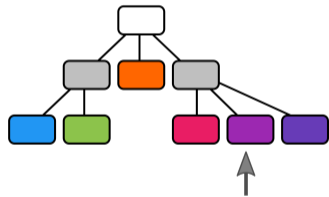
(Gens et al. 2013)



Data-driven structure learning

"Recursive data slicing"

Single variable

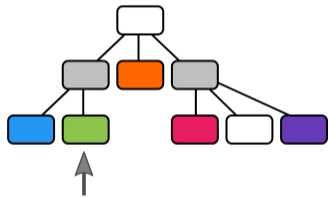


(Gens et al. 2013)

Data-driven structure learning

"Recursive data slicing"

Expand regions with **clustering**



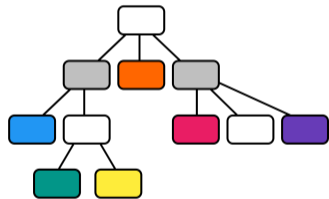
(Gens et al. 2013)

Data-driven structure learning

"Recursive data slicing"

Number of clusters = number of partitions

And so on...

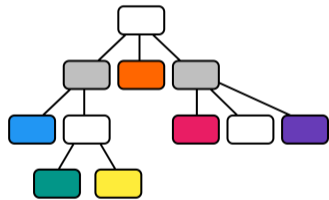


(Gens et al. 2013)

Data-driven structure learning

"Recursive data slicing"

- Stopping conditions: minimal number of features, samples, depth, ...
- Clustering ratios also deliver (initial) parameters
- **Smooth & Decomposable Circuits**
- **Tractable integration**



(Gens et al. 2013)

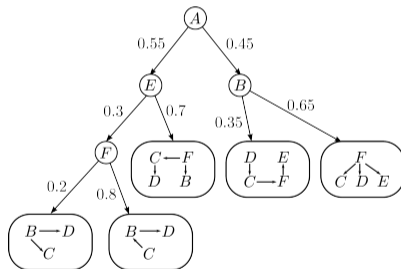
LearnSPN

Selected references

- **ID-SPN** (*Rooshenas et al. 2014*)
- **LearnSPN-b/T/B** (*Vergari et al. 2015*)
- For **heterogeneous data** (*Molina et al. 2018*)
- Using **k-means** (*Butz et al. 2018*) or **SVD** splits (*Adel et al. 2015*)
- Learning **DAGs** (*Dennis et al. 2015; Jaini et al. 2018*)
- **Approximating** independence tests (*Di Mauro et al. 2018*)

Cutset networks

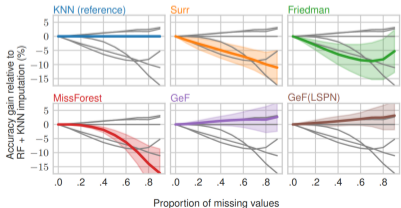
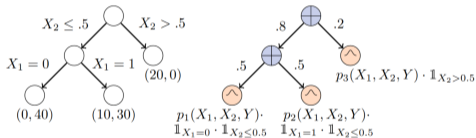
Besides clustering, **decision tree learning** can be used as PC learner. **Cutset networks**, decision trees over simple probabilistic models (Chow-Liu trees) (*Rahman et al. 2014*):



Cutset networks can easily be converted into **smooth, decomposable and deterministic PCs**.

Decision trees as PCs

Also vanilla decision tree learners can be used to learn PCs, by augmenting the leaves with distributions over inputs (*Correia et al. 2020*). Allows to treat **missing features** and **outlier detection**.



Information

Prior Knowledge

domain assumptions
constraints
other models

Data

experimental data
samples
measurements

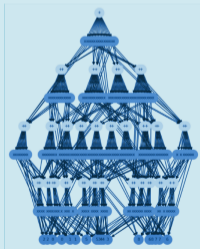
compilation



learning

Circuits

Structure



Parameters

θ, w

decomposability
smoothness
determinism
compatibility

generative
discriminative
Bayesian
credal

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