UCLA Computer Science

STAR AI RESEARCH LAB UCLA

Tractable Probabilistic Circuits

Guy Van den Broeck

Dagstuhl Seminar on Recent Advancements in Tractable Probabilistic Inference - Apr 19, 2022

Outline

1. What are tractable probabilistic circuits?
2. Are these models any good?
3. How far can we push tractable inference?
4. What is their expressive power?

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1. **What are tractable probabilistic circuits?**
2. Are these models any good?
3. How far can we push tractable inference?
4. What is their expressive power?

Fully factorized

NaiveBayes AndOrGraphs PDGs

Trees PSDDs CNets LTMs SPNs NADEs

Thin Junction Trees ACs MADEs MAFs VAEs

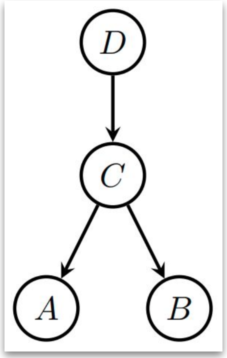
DPPs FVSBNs TACs IAFs NAFs RAEs

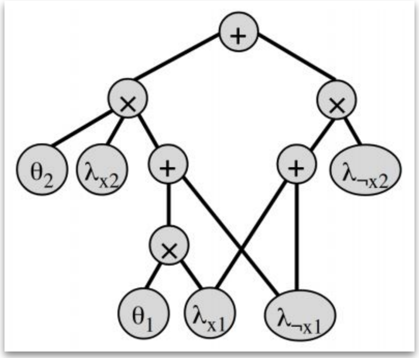
Mixtures BNs NICE FGs GANs

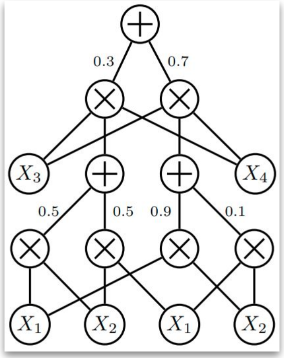
RealNVP MNs

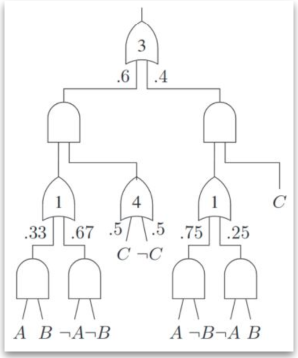
Intractable and *tractable* models

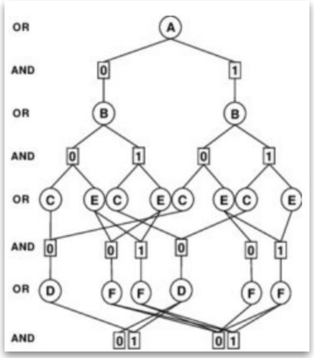
Tractable Probabilistic Models

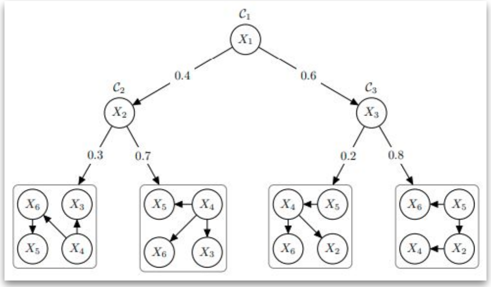


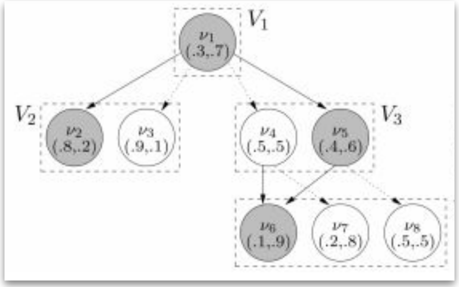


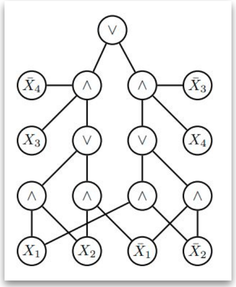


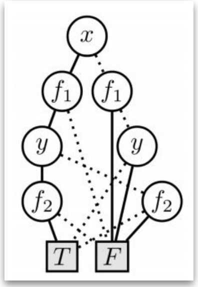


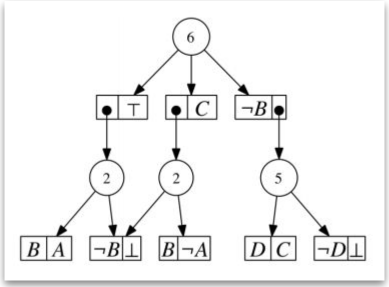




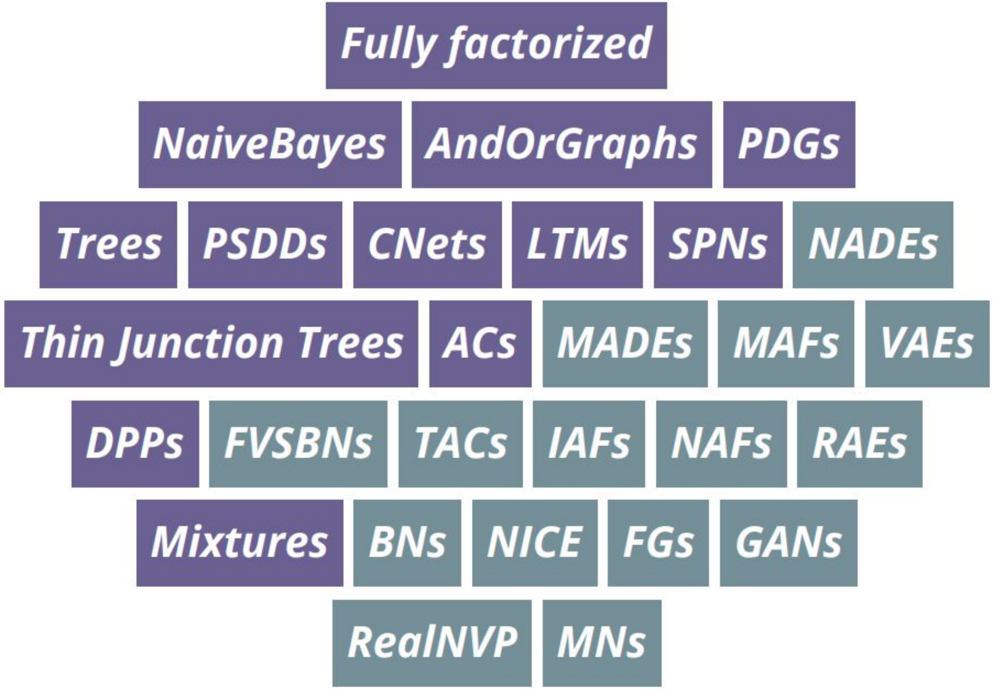








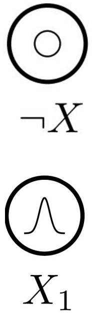
"*Every talk needs a joke and a literature overview slide, not necessarily distinct*"
- after Ron Graham

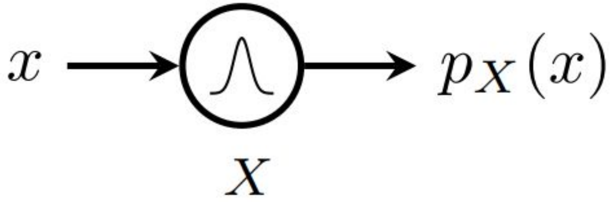


a *unifying framework* for tractable models

Probabilistic circuits

computational graphs that recursively define distributions



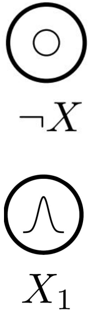


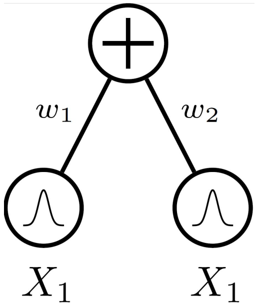
Simple distributions are tractable "black boxes" for:

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

Probabilistic circuits

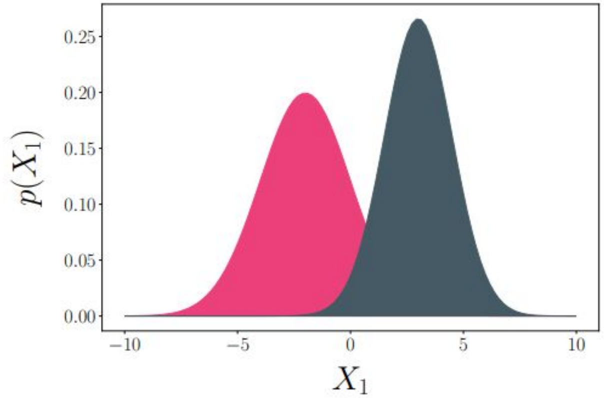
computational graphs that recursively define distributions





$$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$$

⇒ *mixtures*



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

Probabilistic circuits

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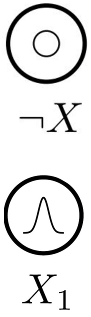
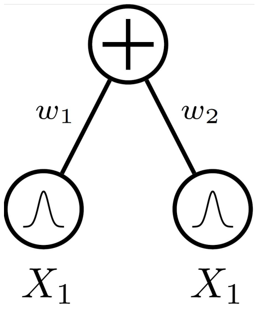
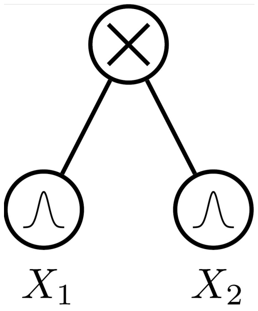
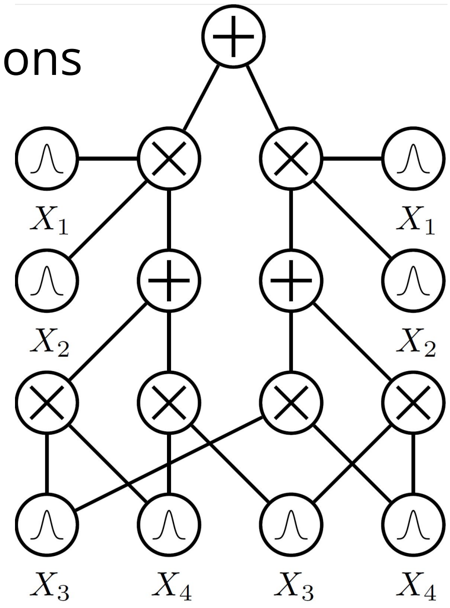








$$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$$

⇒ *mixtures*

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

⇒ *factorizations*

Tractable Probabilistic Inference

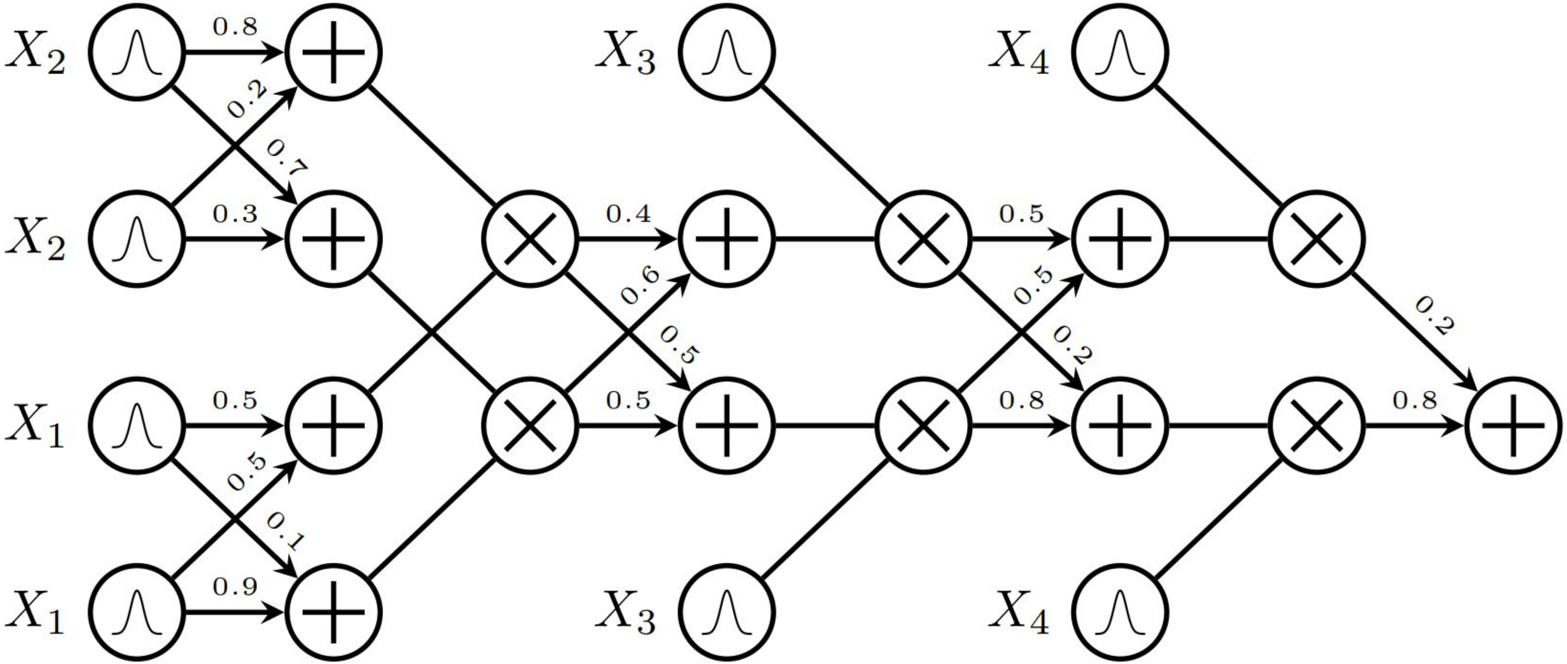
A class of queries $\mathcal{Q}$ *is* tractable *on a family of probabilistic models* $\mathcal{M}$
iff for any query $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$
exactly *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\text{poly}(|\mathbf{m}|))$.

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

$\Rightarrow$ *Note: if* $\mathcal{M}$ *is compact in the number of random variables* $\mathbf{X}$*, that is,*
$|\mathbf{m}| \in O(\text{poly}(|\mathbf{X}|))$*, then query time is* $O(\text{poly}(|\mathbf{X}|))$.

Likelihood

$$p(X_1 = \mathbf{-1.85}, X_2 = \mathbf{0.5}, X_3 = \mathbf{-1.3}, X_4 = \mathbf{0.2})$$



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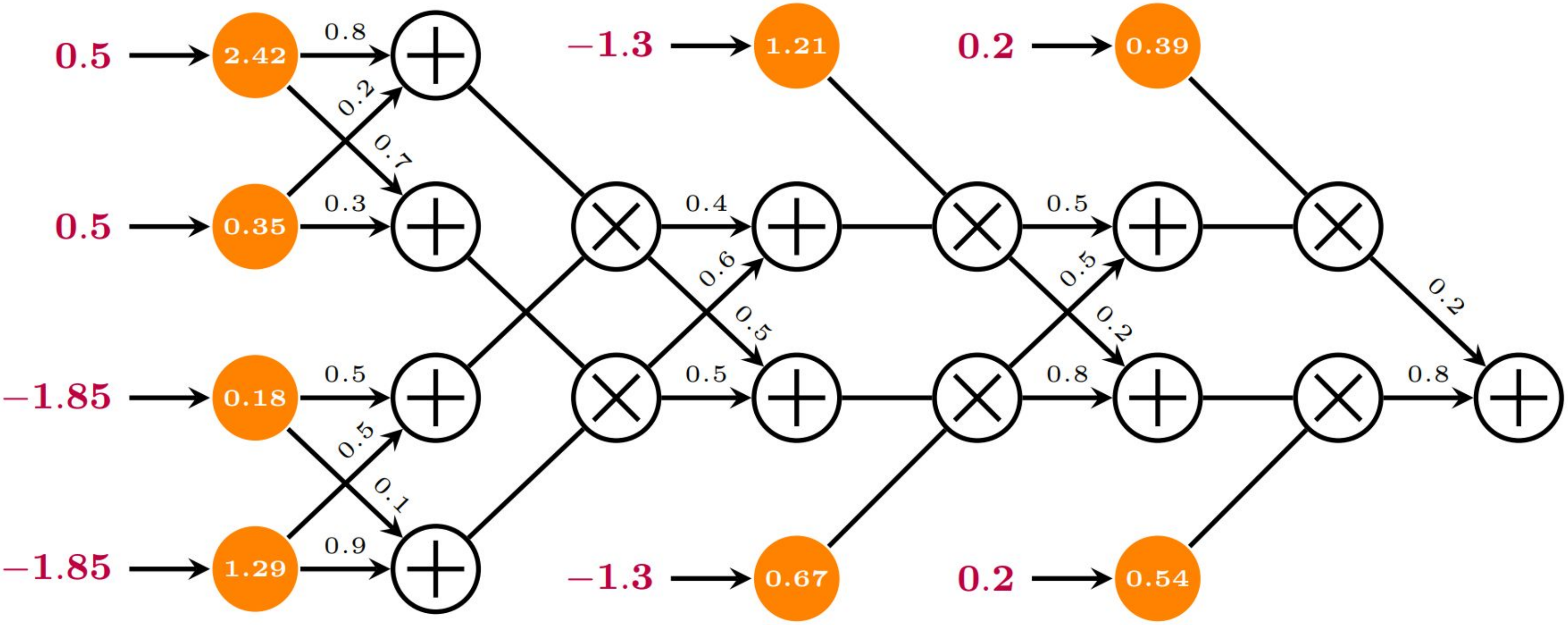

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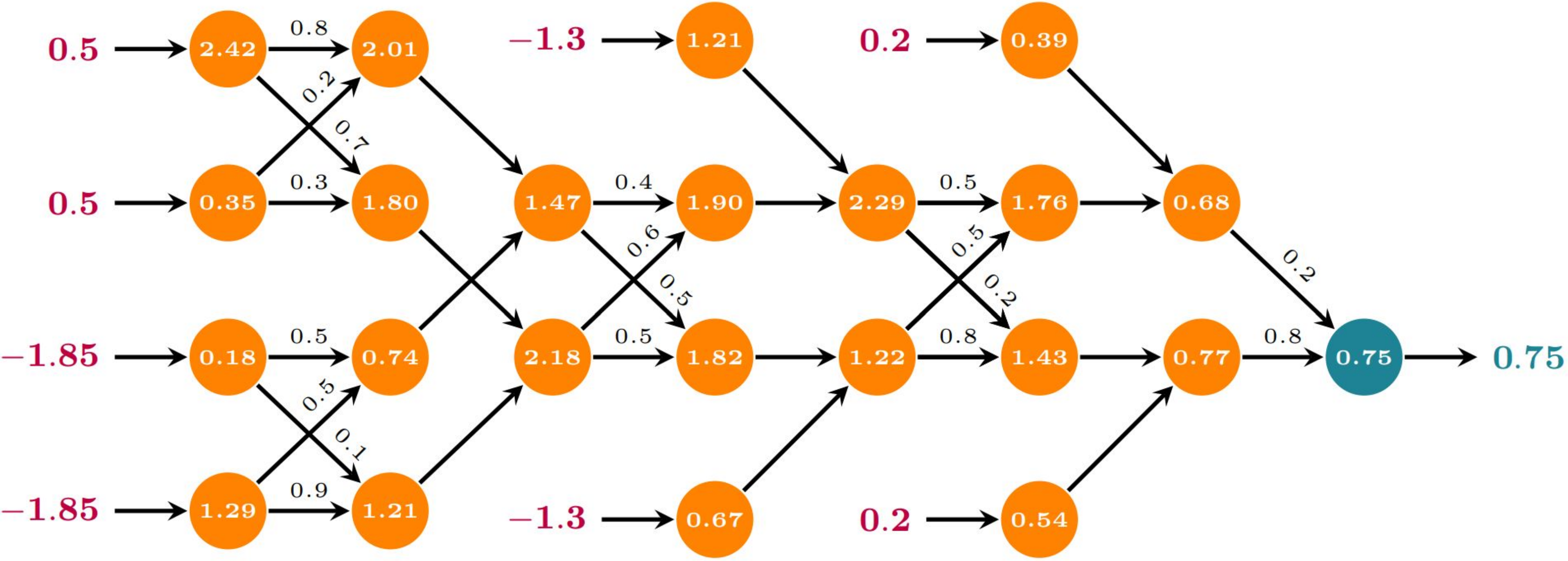
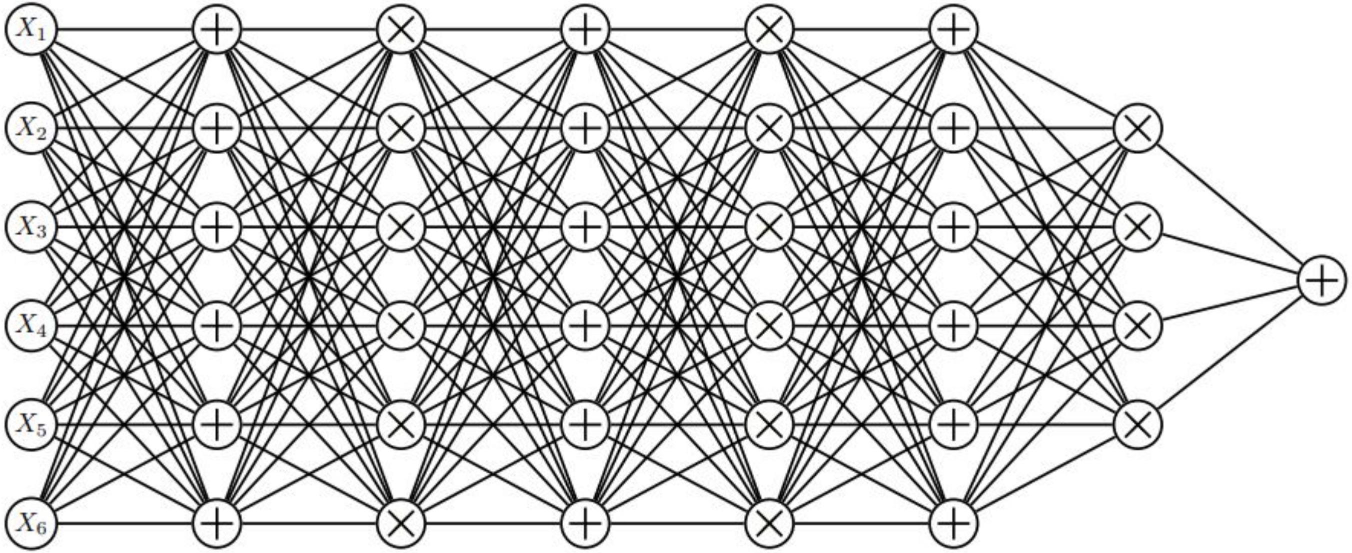


Just sum, products and distributions?



just arbitrarily compose them like a neural network!

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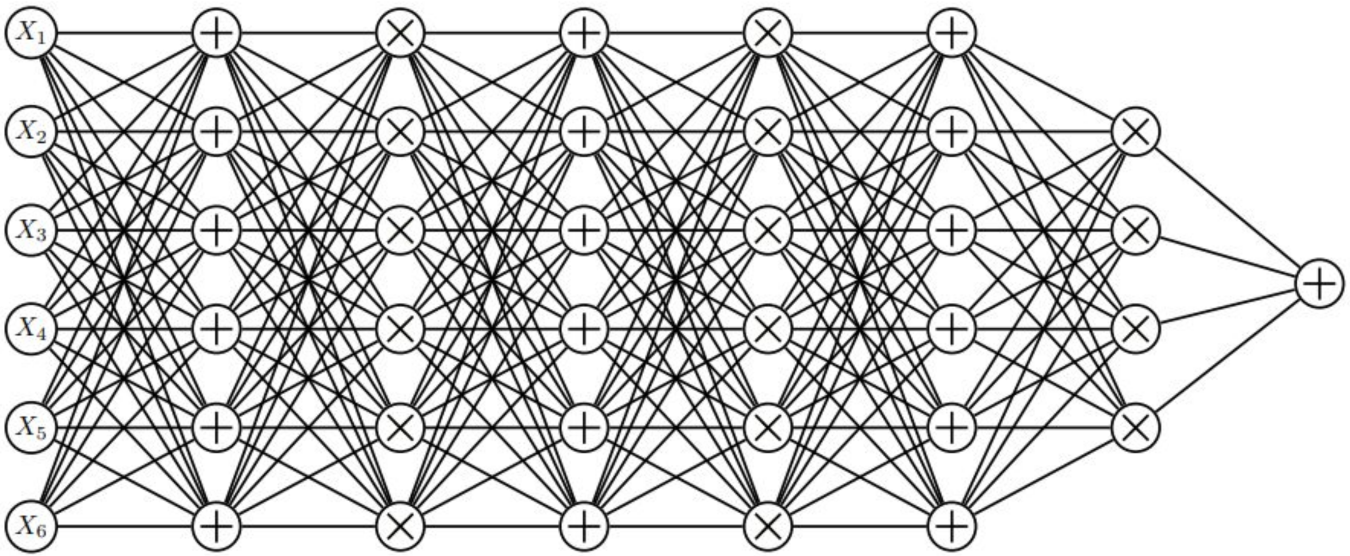


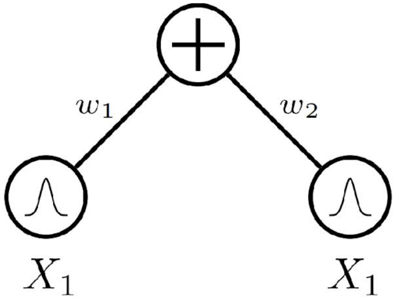
~~***just arbitrarily compose them like a neural network!***~~

⇒ structural constraints needed for tractability

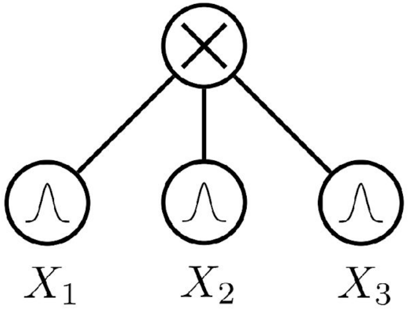
Tractable marginals

A sum node is ***smooth*** if its children depend on the same set of variables.

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



smooth circuit



decomposable circuit

Darwiche and Marquis, “A Knowledge Compilation Map”, 2002

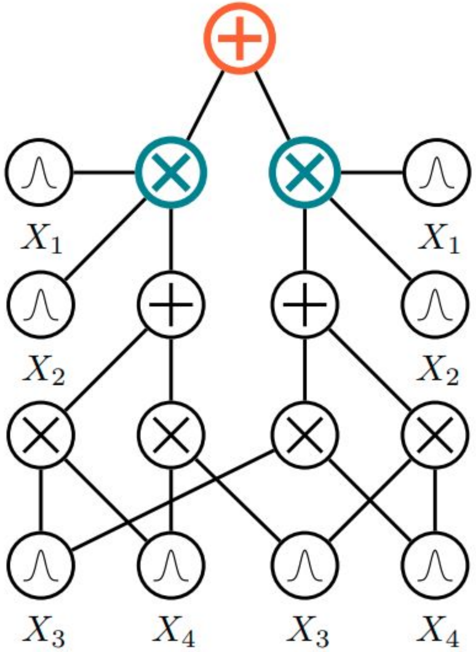
Smoothness + decomposability = tractable MAR

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*



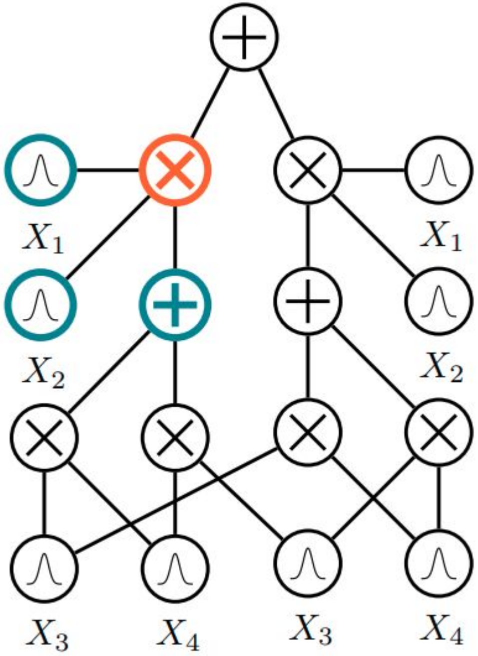
[Darwiche & Marquis JAIR 2001, Poon & Domingos UAI11]

Smoothness + decomposability = tractable MAR

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

$$\int\int\int p(\mathbf{x},\mathbf{y},\mathbf{z})d\mathbf{x}d\mathbf{y}d\mathbf{z} =$$
$$= \int\int\int p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})d\mathbf{x}d\mathbf{y}d\mathbf{z} =$$
$$= \int p(\mathbf{x})d\mathbf{x} \int p(\mathbf{y})d\mathbf{y} \int p(\mathbf{z})d\mathbf{z}$$

$\Rightarrow$ *integrals decompose into easier ones*



Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

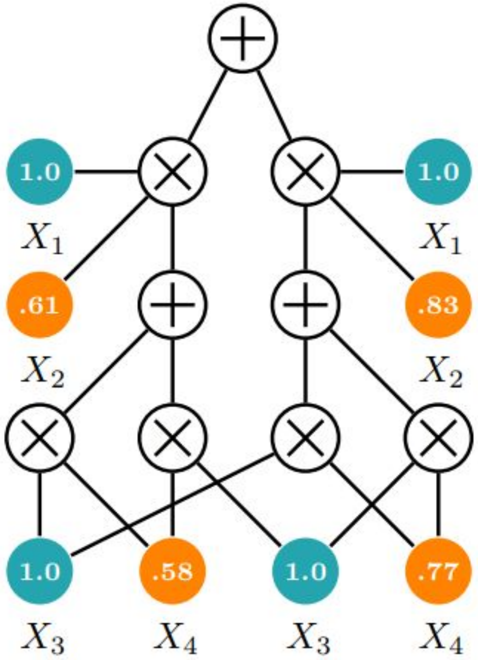
$\Rightarrow$ *linear in circuit size!*

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

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

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

- leafs over X_2 and X_4 output ***EVI***
- feedforward evaluation (bottom-up)



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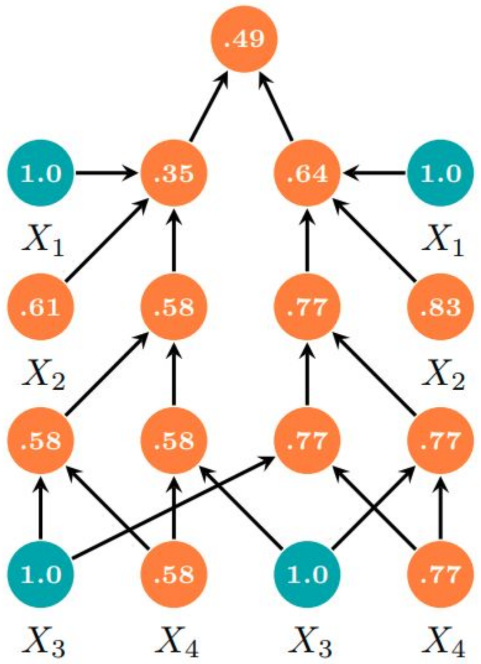
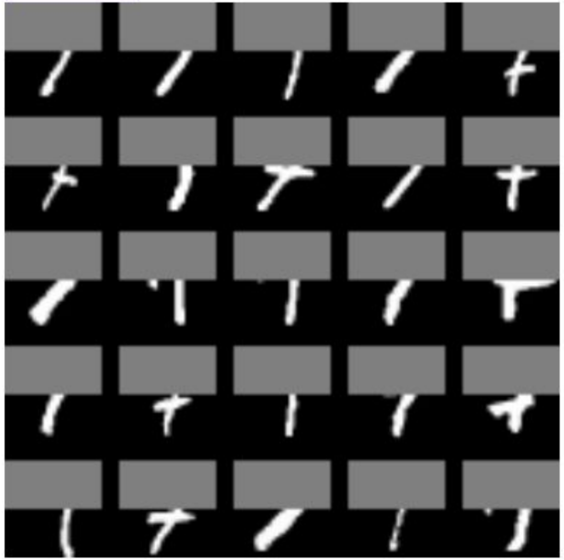


Tractable MAR on PCs (Einsum Networks)

EVI $10,958.72\,\text{nats}$

MAR $5,387.55\,\text{nats}$



Peharz et al., "Einsum Networks: Fast and Scalable Learning of Tractable Probabilistic Circuits", 2020

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

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

$\Longrightarrow$ *MAP for latent variable models is* **intractable** *[Conaty et al. 2017]*

Outline

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Where do architectures come from?

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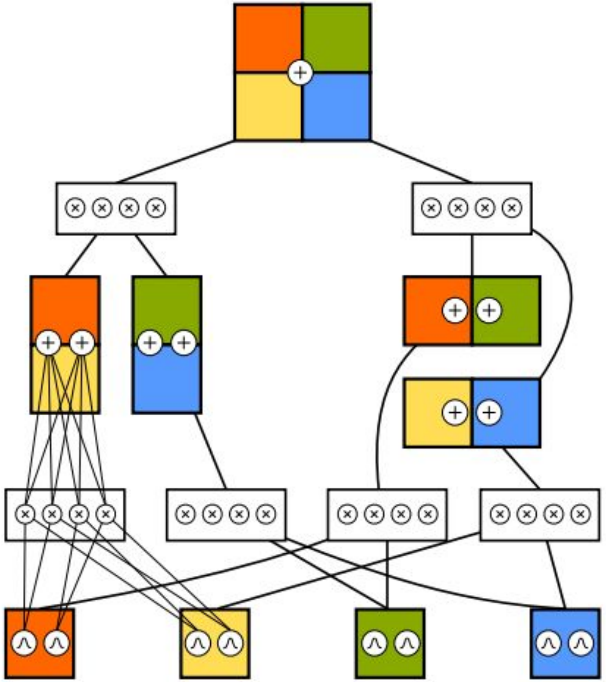

Poon and Domingos, "Sum-Product Networks: a New Deep Architecture", 2011

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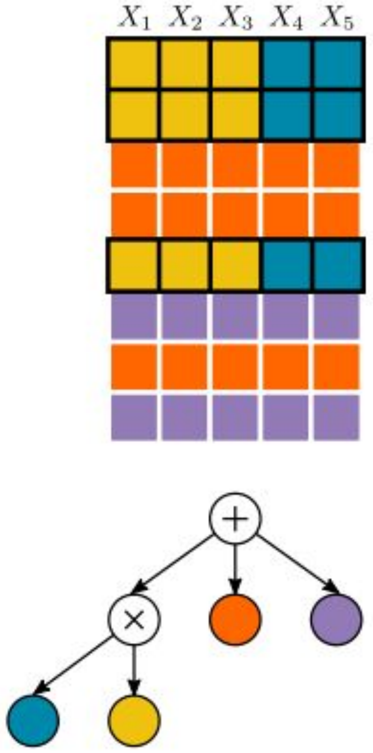

Gens and Domingos, "Learning the Structure of Sum-Product Networks", 2013

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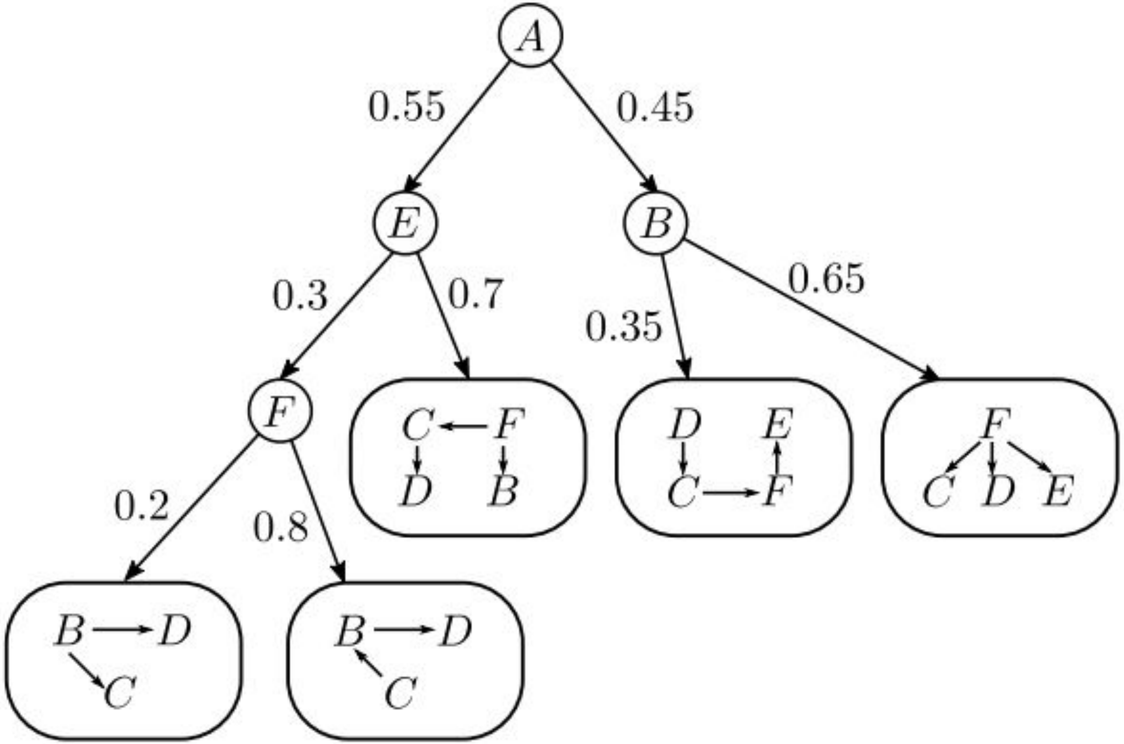
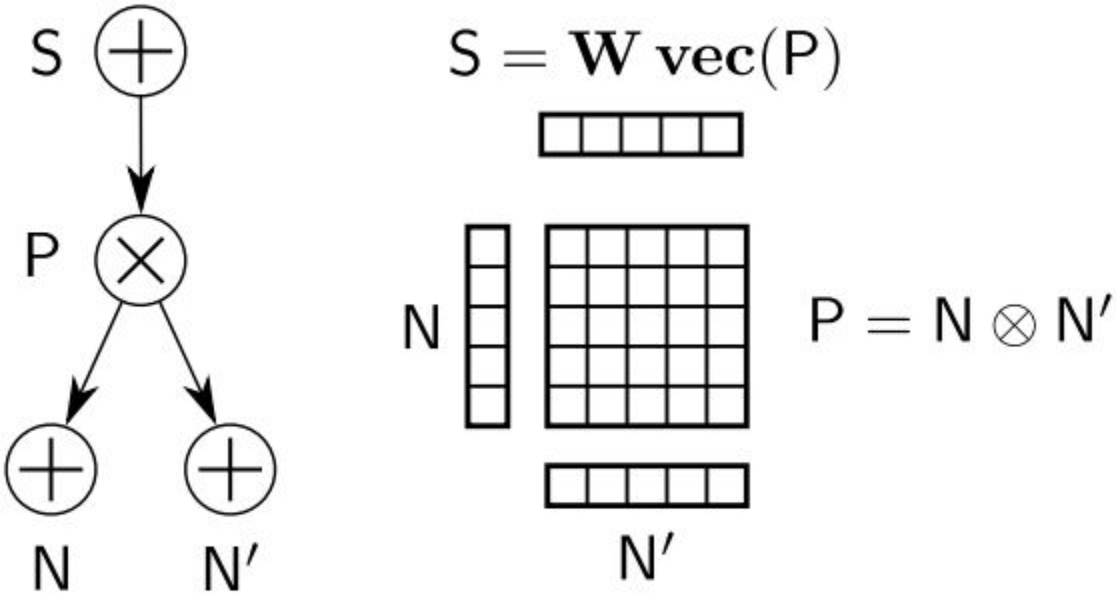


[Rahman et al. 2014]

Where do architectures come from?

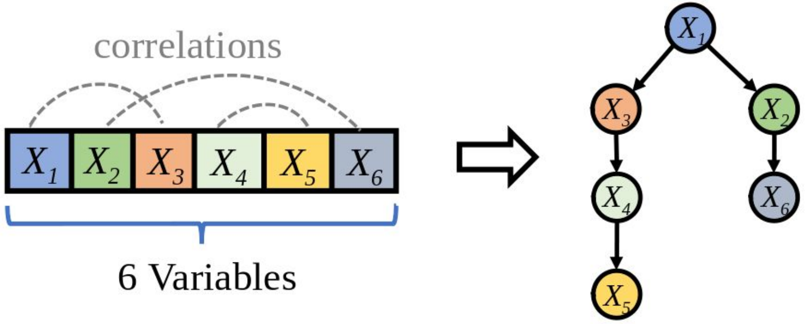


Einsum Networks: Fast and Scalable Learning of Tractable Probabilistic Circuits

Learning Expressive Probabilistic Circuits

Hidden Chow-Liu Trees

Learned **CLT structure** captures strong pairwise dependencies



Anji Liu and Guy Van den Broeck. Tractable Regularization of Probabilistic Circuits, *NeurIPS*, 2021.

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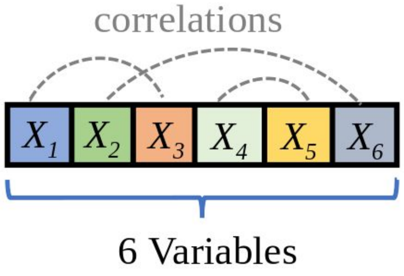

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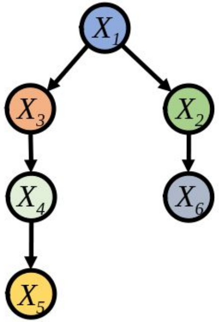
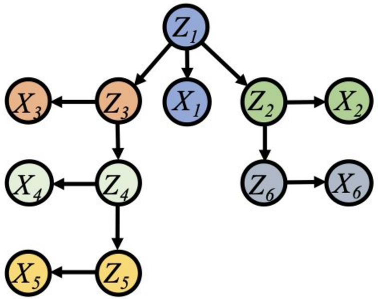


Learned **HCLT structure**

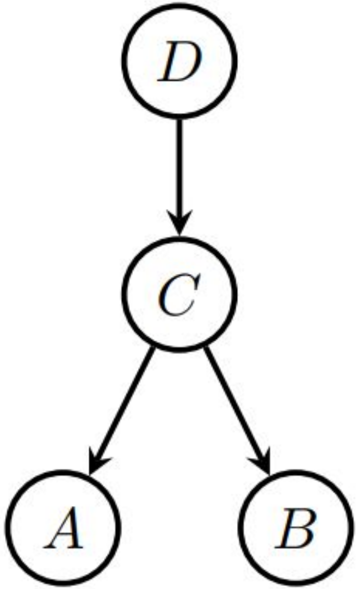


Compile into an equivalent PC

Anji Liu and Guy Van den Broeck. Tractable Regularization of Probabilistic Circuits, *NeurIPS*, 2021.

From BN trees to circuits

via compilation



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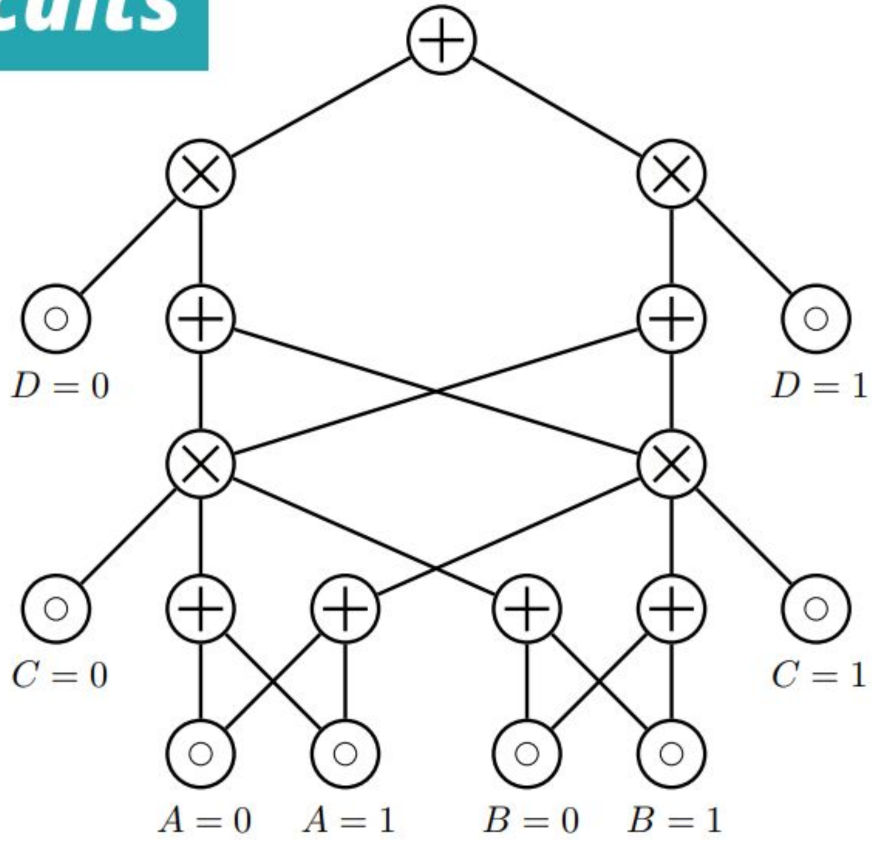

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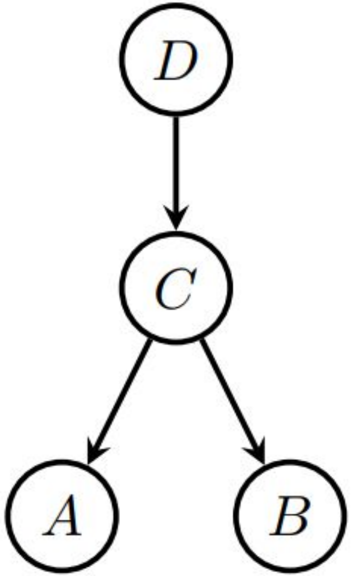
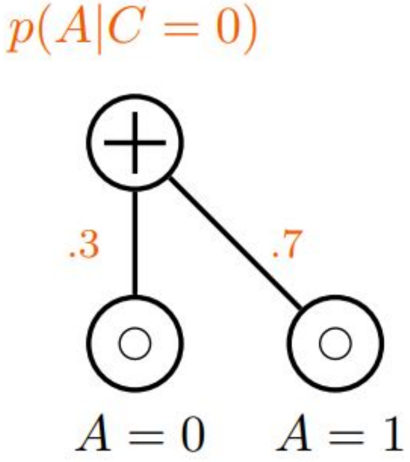


...compile a leaf CPT



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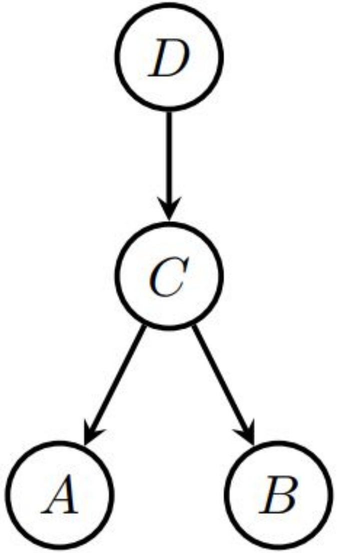
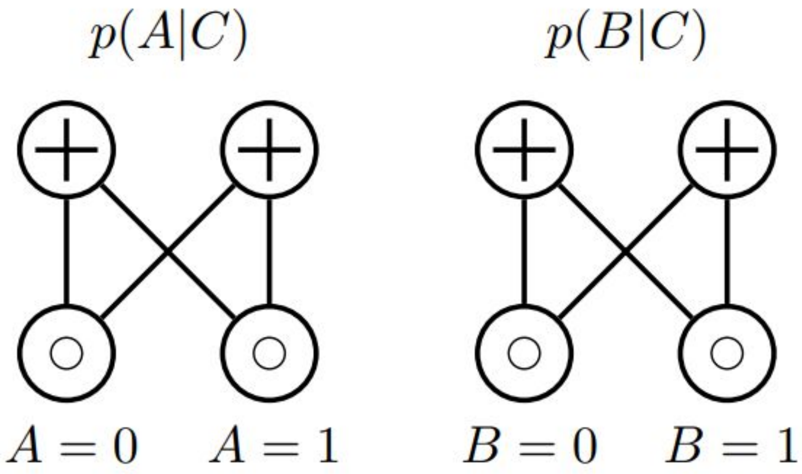


...compile a leaf CPT...for all leaves...



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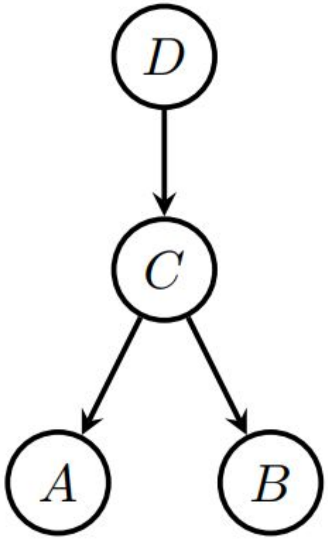
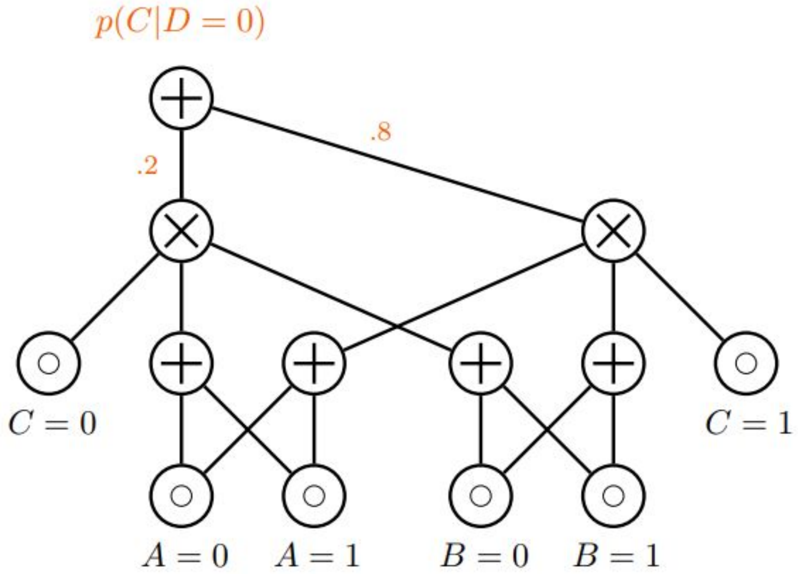


...and recurse over parents...



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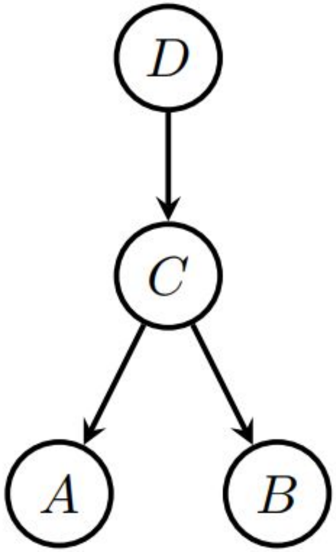

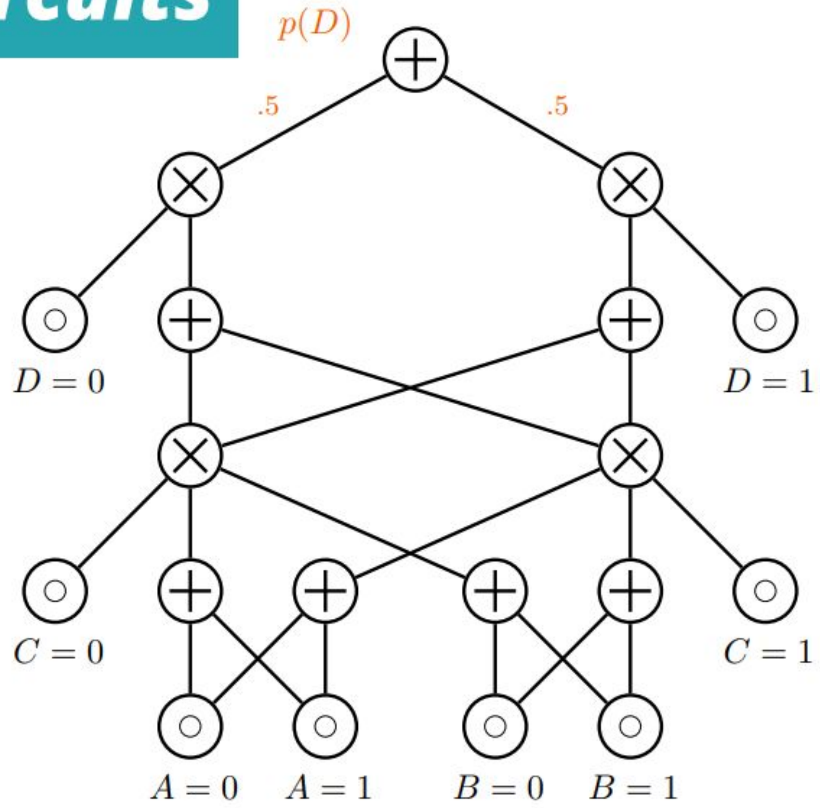

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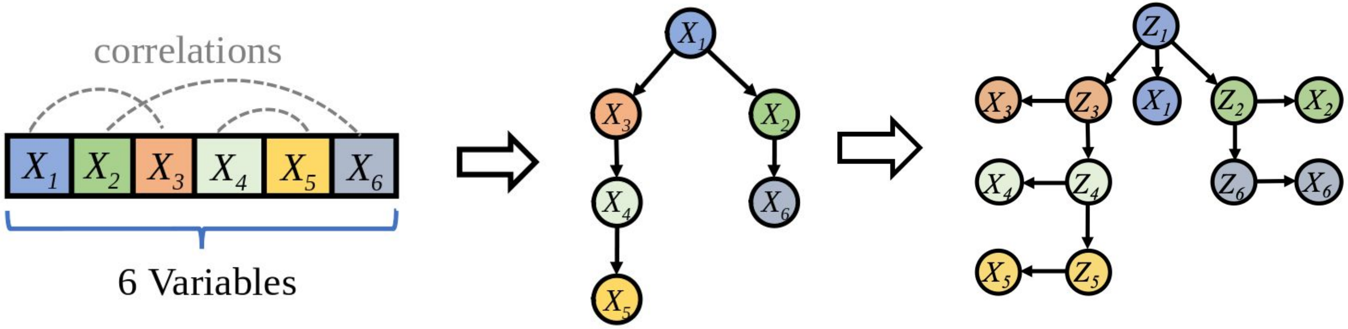
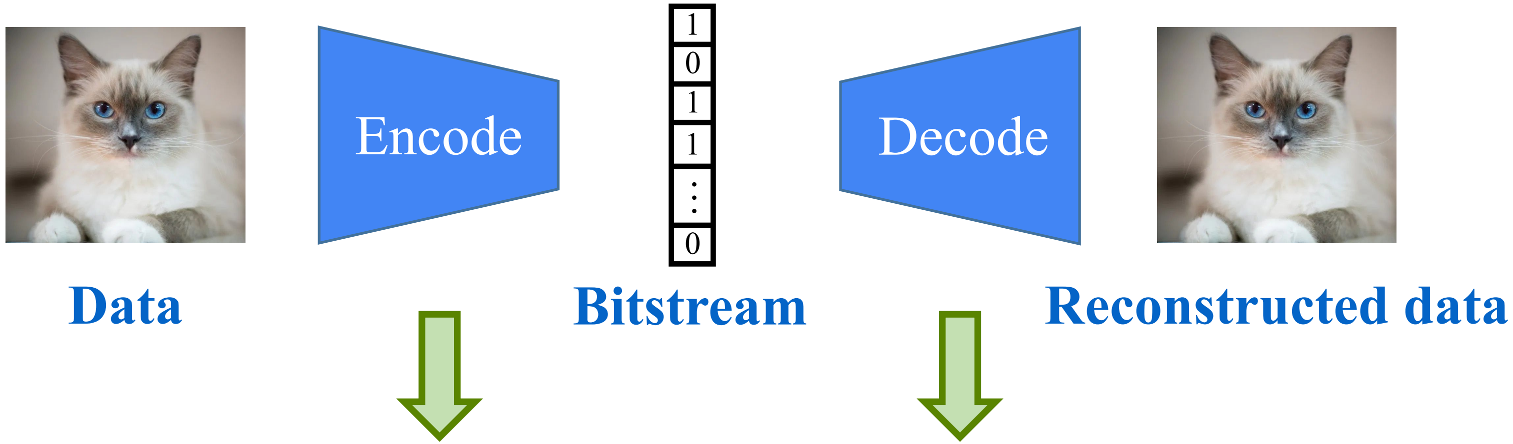


⇨ **Compile** into an equivalent PC

⇨ Mini-batch Stochastic **Expectation Maximization**

Anji Liu and Guy Van den Broeck. Tractable Regularization of Probabilistic Circuits, *NeurIPS*, 2021.

Lossless Data Compression



Expressive probabilistic model $p(\boldsymbol{x})$ ⇨ Determines the theoretical limit of compression rate

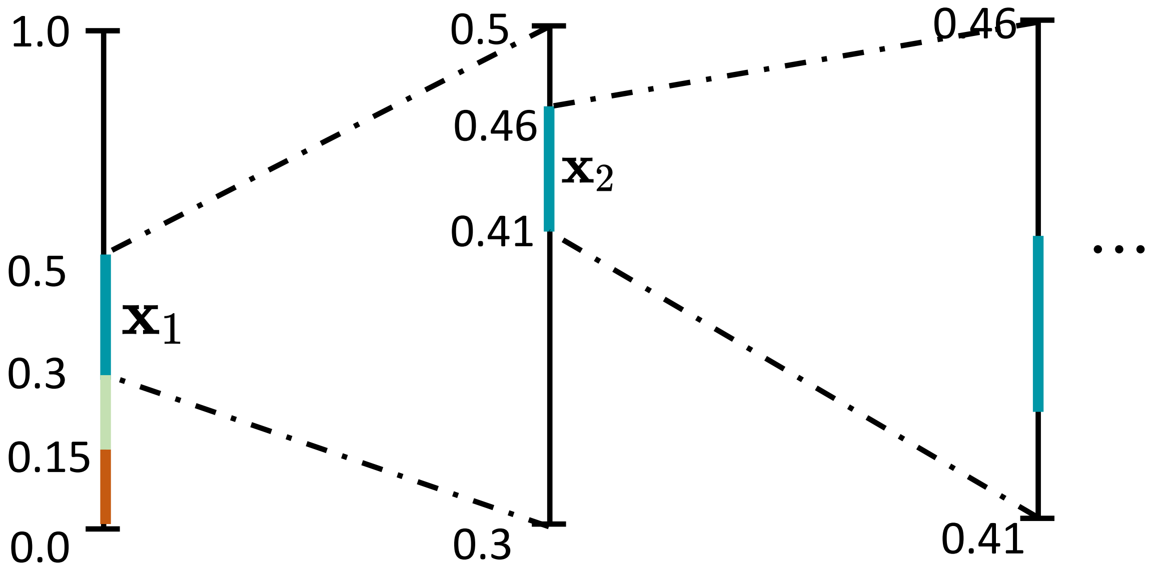
+

Efficient coding algorithm ⇨ How close we can approach the theoretical limit

Anji Liu, Stephan Mandt and Guy Van den Broeck. Lossless Compression with Probabilistic Circuits, 2021.

A Typical Streaming Code – Arithmetic Coding

We want to compress a set of variables (e.g., pixels, letters) $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_k\}$



Compress $\mathbf{x}_1$ with $-\log p(\mathbf{x}_1)$ bits

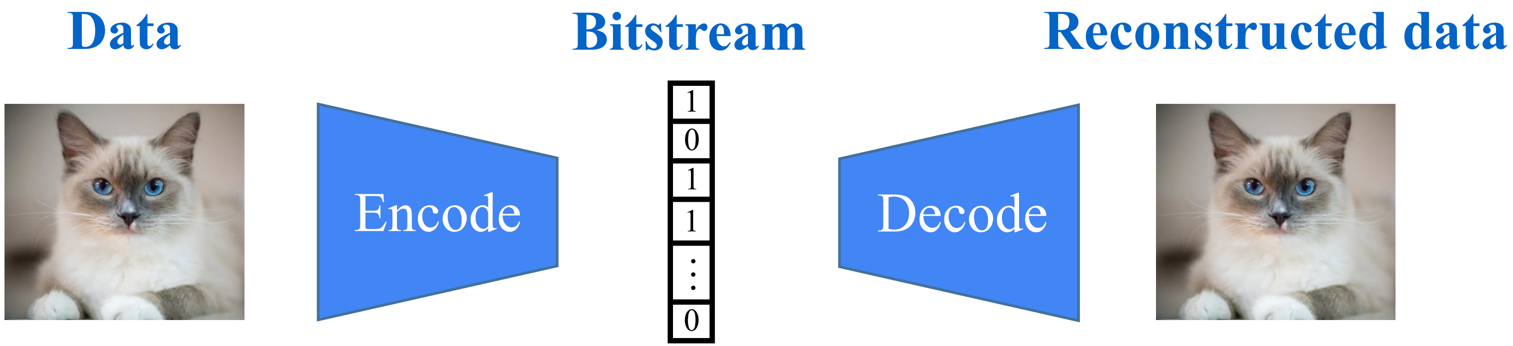
Compress $\mathbf{x}_2$ with $-\log p(\mathbf{x}_2|\mathbf{x}_1)$ bits

Compress $\mathbf{x}_3$ with $-\log p(\mathbf{x}_3|\mathbf{x}_1, \mathbf{x}_2)$ bits

Need to compute

$$p(X_1 < x_1)$$
$$p(X_1 \leq x_1)$$
$$p(X_2 < x_2|x_1)$$
$$p(X_2 \leq x_2|x_1)$$
$$p(X_3 < x_3|x_1, x_2)$$
$$p(X_3 \leq x_3|x_1, x_2)$$
$$\vdots$$

Lossless Neural Compression with Probabilistic Circuits



Probabilistic Circuits

- Expressive → SoTA likelihood on MNIST.
- Fast → Time complexity of en/decoding is **O(|p| log(D))**, where D is the # variables and |p| is the size of the PC.

Arithmetic Coding:

$$p(X_1 < x_1)$$
$$p(X_1 \leq x_1)$$
$$p(X_2 < x_2 | x_1)$$
$$p(X_2 \leq x_2 | x_1)$$
$$p(X_3 < x_3 | x_1, x_2)$$
$$p(X_3 \leq x_3 | x_1, x_2)$$
$$\vdots$$

Anji Liu, Stephan Mandt and Guy Van den Broeck. Lossless Compression with Probabilistic Circuits, 2021.

Lossless Neural Compression with Probabilistic Circuits

SoTA compression rates

Dataset	HCLT (ours)	IDF	BitSwap	BB-ANS	JPEG2000	WebP	McBits
MNIST	**1.24** (1.20)	1.96 (1.90)	1.31 (1.27)	1.42 (1.39)	3.37	2.09	(1.98)
FashionMNIST	3.37 (3.34)	3.50 (3.47)	**3.35** (3.28)	3.69 (3.66)	3.93	4.62	(3.72)
EMNIST (Letter)	**1.84** (1.80)	2.02 (1.95)	1.90 (1.84)	2.29 (2.26)	3.62	3.31	(3.12)
EMNIST (ByClass)	**1.89** (1.85)	2.04 (1.98)	1.91 (1.87)	2.24 (2.23)	3.61	3.34	(3.14)

Compress and decompress 5-40x faster than NN methods with similar bitrates

Method	# parameters	Theoretical bpd	Codeword bpd	Comp. time (s)	Decomp. time (s)
PC (HCLT, $M=16$)	3.3M	1.26	1.30	9	44
PC (HCLT, $M=24$)	5.1M	1.22	1.26	15	86
PC (HCLT, $M=32$)	7.0M	1.20	1.24	26	142
IDF	24.1M	1.90	1.96	288	592
BitSwap	2.8M	1.27	1.31	578	326

Anji Liu, Stephan Mandt and Guy Van den Broeck. Lossless Compression with Probabilistic Circuits, 2021.

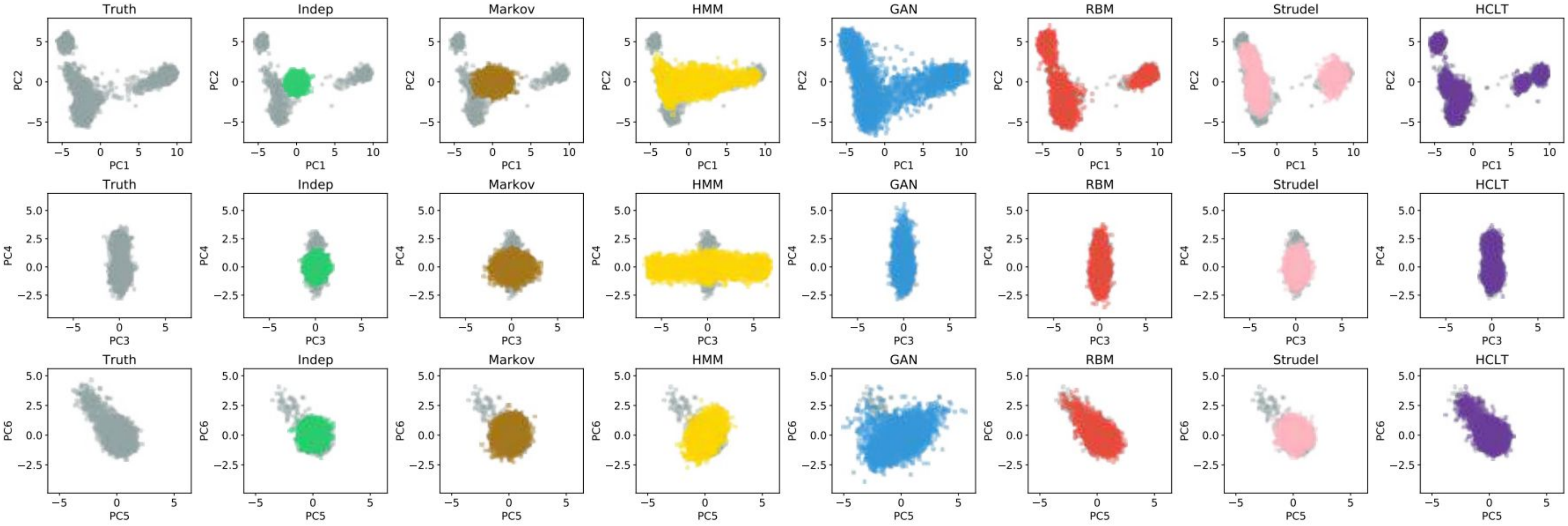
Lossless Neural Compression with Probabilistic Circuits

Can be effectively combined with Flow models to achieve better generative performance

Model	CIFAR10	ImageNet32	ImageNet64
RealNVP	3.49	4.28	3.98
Glow	3.35	4.09	3.81
IDF	3.32	4.15	3.90
IDF++	**3.24**	4.10	3.81
PC+IDF	3.28	**3.99**	**3.71**

Anji Liu, Stephan Mandt and Guy Van den Broeck. Lossless Compression with Probabilistic Circuits, 2021.

Tractable and expressive generative models of genetic variation data

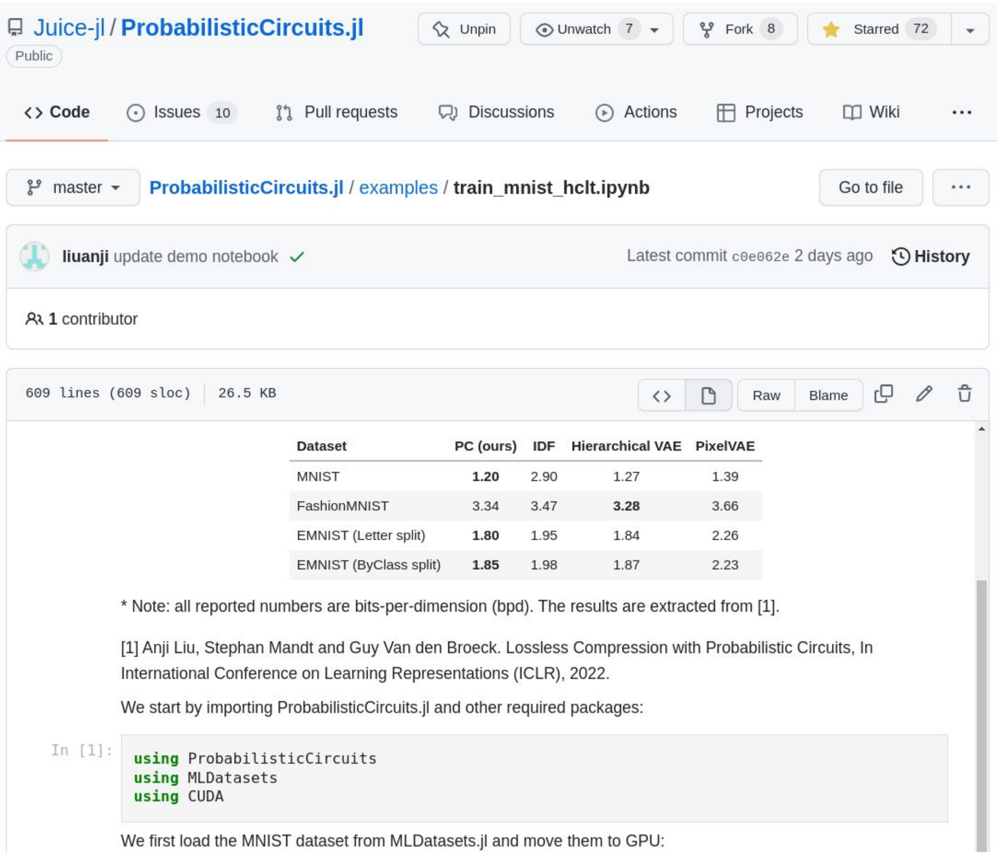


Meihua Dang , Anji Liu , Xinzhu Wei , Sriram Sankararaman, and Guy Van den Broeck, Tractable and expressive generative models of genetic variation data, RECOMB 2022

Text data

Dataset	PC	Bipartite flow	AF/SCF	IAF/SCF
Penn Treebank	**1.23**	1.38	1.46	1.63

Training SotA likelihood full MNIST probabilistic circuit model in ~7 minutes on GPU:
https://github.com/Juice-jl/ProbabilisticCircuits.jl/blob/master/examples/train_mnist_hclt.ipynb



Juice-jl / ProbabilisticCircuits.jl
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master | ProbabilisticCircuits.jl / examples / train_mnist_hclt.ipynb | Go to file | ...

liuanji update demo notebook ✓ Latest commit c0e062e 2 days ago History

1 contributor

609 lines (609 sloc) | 26.5 KB | Raw | Blame

Dataset	PC (ours)	IDF	Hierarchical VAE	PixelVAE
MNIST	**1.20**	2.90	1.27	1.39
FashionMNIST	3.34	3.47	**3.28**	3.66
EMNIST (Letter split)	**1.80**	1.95	1.84	2.26
EMNIST (ByClass split)	**1.85**	1.98	1.87	2.23

* Note: all reported numbers are bits-per-dimension (bpd). The results are extracted from [1].

[1] Anji Liu, Stephan Mandt and Guy Van den Broeck. Lossless Compression with Probabilistic Circuits, In International Conference on Learning Representations (ICLR), 2022.

We start by importing ProbabilisticCircuits.jl and other required packages:

In [1]:

```
using ProbabilisticCircuits
using MLDatasets
using CUDA
```

We first load the MNIST dataset from MLDatasets.jl and move them to GPU:

Fully factorized

NaiveBayes AndOrGraphs PDGs

Trees PSDDs CNets LTMs SPNs NADEs

Thin Junction Trees ACs MADEs MAFs VAEs

DPPs FVSBNs TACs IAFs NAFs RAEs

Mixtures BNs NICE FGs GANs

RealNVP MNs

Expressive models without *compromises*

Outline

1. What are tractable probabilistic circuits?
2. Are these models any good?
3. **How far can we push tractable inference?**
4. What is their expressive power?

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

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

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

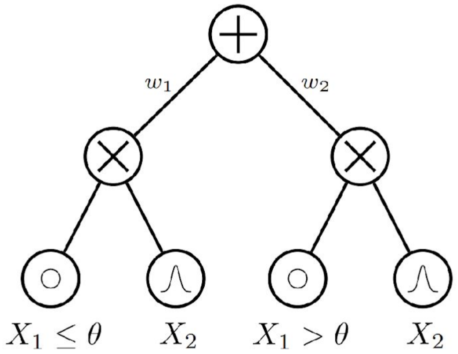
since for a sum node we are marginalizing out a latent variable

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

$\Rightarrow$ *MAP for latent variable models is* **intractable** *[Conaty et al. 2017]*

Determinism

A sum node is ***deterministic*** if only one of its children outputs non-zero for any input



deterministic circuit

$\Rightarrow$ *allows* ***tractable MAP*** *inference*

$$argmax_{\boldsymbol{x}}\, p(\boldsymbol{x})$$

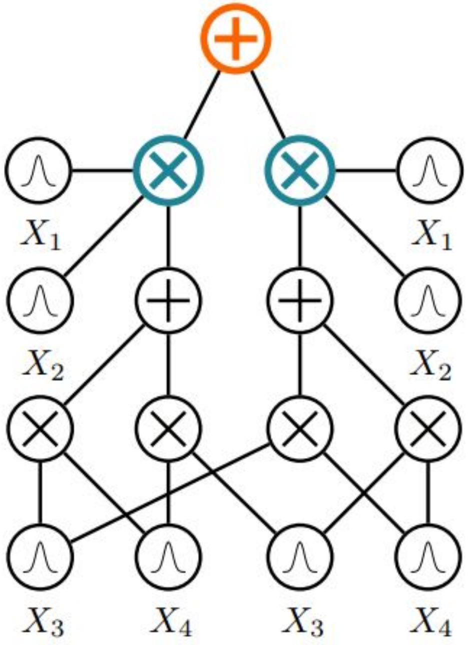
Darwiche and Marquis, “A Knowledge Compilation Map”, 2002

Determinism + decomposability = tractable MAP

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

$$\max_{\mathbf{q}} \boldsymbol{p}(\mathbf{q}, \mathbf{e}) = \max_{\mathbf{q}} \sum_i w_i \boldsymbol{p}_i(\mathbf{q}, \mathbf{e})$$
$$= \max_{\mathbf{q}} \max_i w_i \boldsymbol{p}_i(\mathbf{q}, \mathbf{e})$$
$$= \max_i \max_{\mathbf{q}} w_i \boldsymbol{p}_i(\mathbf{q}, \mathbf{e})$$

$\Rightarrow$ *one non-zero child term, thus sum is max*

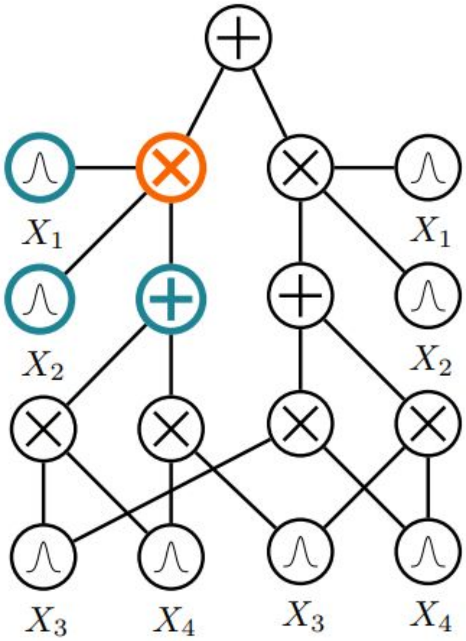


Determinism + decomposability = tractable MAP

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):

$$\max_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e}) = \max_{\mathbf{q}} p(\mathbf{q},\mathbf{e})$$
$$= \max_{\mathbf{q_x},\mathbf{q_y}} p(\mathbf{q_x},\mathbf{e_x},\mathbf{q_y},\mathbf{e_y})$$
$$= \max_{\mathbf{q_x}} p(\mathbf{q_x},\mathbf{e_x}) \cdot \max_{\mathbf{q_y}} p(\mathbf{q_y},\mathbf{e_y})$$

$\Longrightarrow$ *solving optimization independently*

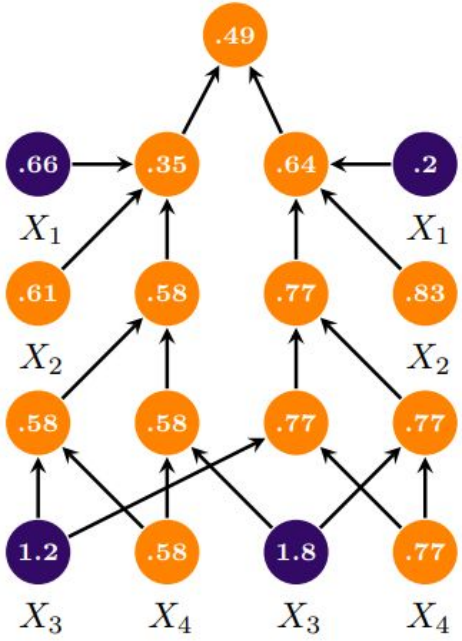


Determinism + **decomposability** = **tractable MAP**

Evaluating the circuit twice:
bottom-up and ***top-down*** $\Rightarrow$ *still linear in circuit size!*

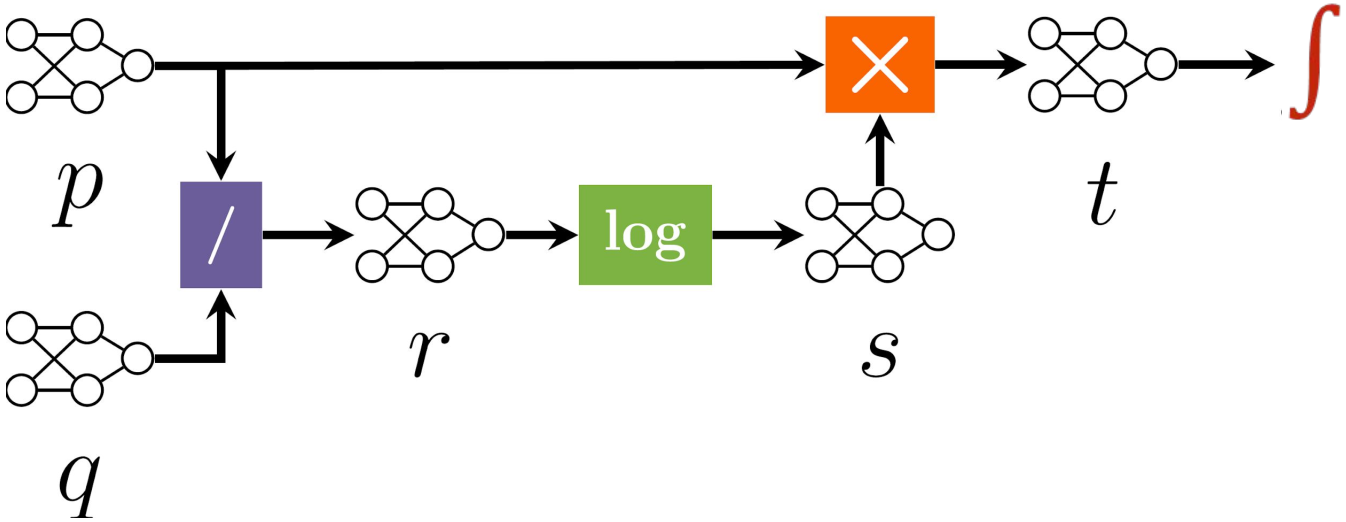
E.g., for $\text{argmax}_{x_1,x_3} p(x_1, x_3 \mid x_2, x_4)$:

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



Queries as pipelines: KLD

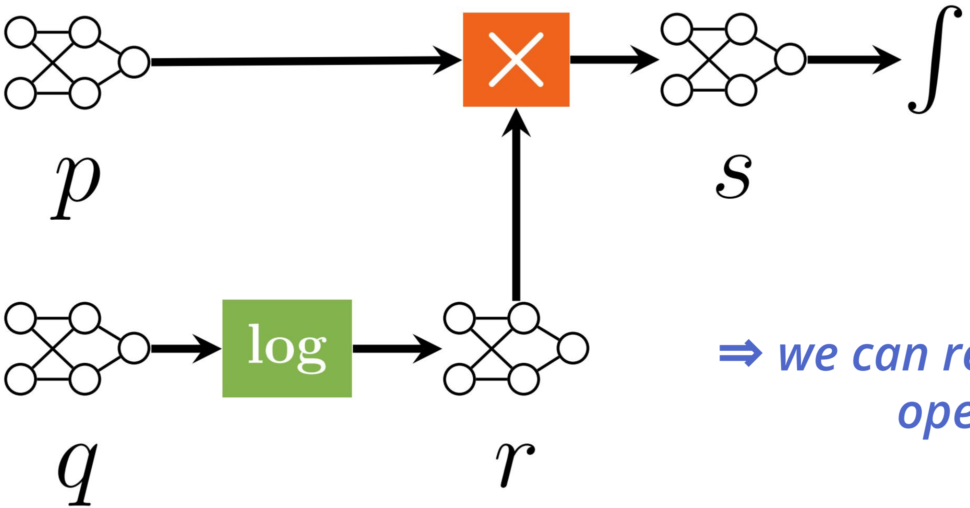
$$\mathbb{KLD}(p \parallel q) = \int p(\boldsymbol{x}) \times \log((p(\boldsymbol{x})/q(\boldsymbol{x}))d\boldsymbol{X}$$



Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Queries as pipelines: Cross Entropy

$$H(p, q) = \int p(\boldsymbol{x}) \times \log(q(\boldsymbol{x}))d\boldsymbol{X}$$



⇒ *we can reuse the operations!*

Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Operation		Tractability	
		Input conditions	Output conditions
LOG	$\log(p)$	Sm, Dec, Det	Sm, Dec

smooth, decomposable, deterministic

smooth, decomposable

Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Tractable circuit operations

Operation		Tractability: Input properties	Tractability: Output properties	Hardness
SUM	$\theta_1 p + \theta_2 q$	(+Cmp)	(+SD)	NP-hard for Det output
PRODUCT	$p \cdot q$	Cmp (+Det, +SD)	Dec (+Det, +SD)	#P-hard w/o Cmp
POWER	$p^n, n \in \mathbb{N}$	SD (+Det)	SD (+Det)	#P-hard w/o SD
	$p^\alpha, \alpha \in \mathbb{R}$	Sm, Dec, Det (+SD)	Sm, Dec, Det (+SD)	#P-hard w/o Det
QUOTIENT	p/q	Cmp; q Det (+p Det,+SD)	Dec (+Det,+SD)	#P-hard w/o Det
LOG	$\log(p)$	Sm, Dec, Det	Sm, Dec	#P-hard w/o Det
EXP	$\exp(p)$	linear	SD	#P-hard

Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Inference by tractable operations

systematically derive tractable inference algorithm of complex queries

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

Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Even harder queries

Marginal MAP

Given a set of query variables $\boldsymbol{Q} \subset \boldsymbol{X}$ and evidence $\boldsymbol{e}$,

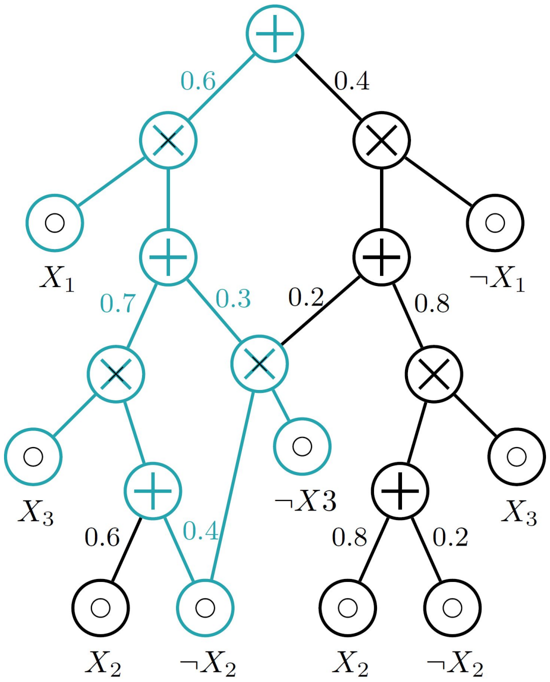
find: $argmax_{\boldsymbol{q}}\, p(\boldsymbol{q}|\boldsymbol{e})$

⇒ *i.e. MAP of a marginal distribution on* ***Q***

! *NP^{PP}-complete for PGMs*

! ***NP-hard*** *even for PCs tractable for marginals, MAP & entropy*

Pruning circuits



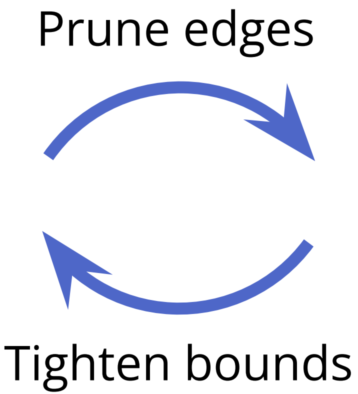
Any parts of circuit not relevant for MMAP state can be pruned away

e.g. $p(X_1 = 1, X_2 = 0)$

We can find such edges in *linear time*

YooJung Choi, Tal Friedman and Guy Van den Broeck. Solving Marginal MAP Exactly by Probabilistic Circuit Transformations, 2021.

Iterative MMAP solver



Dataset	runtime (# solved) search	runtime (# solved) pruning
NLTCS	**0.01** (10)	0.63 (10)
MSNBC	**0.03** (10)	0.73 (10)
KDD	**0.04** (10)	0.68 (10)
Plants	2.95 (10)	**2.72** (10)
Audio	2041.33 (6)	**13.70 (10)**
Jester	2913.04 (2)	**14.74 (10)**
Netflix	– (0)	**47.18 (10)**
Accidents	109.56 (10)	**15.86** (10)
Retail	**0.06** (10)	0.81 (10)
Pumsb-star	2208.27 (7)	**20.88 (10)**
DNA	– (0)	**505.75 (9)**
Kosarek	48.74 (10)	**3.41** (10)
MSWeb	1543.49 (10)	**1.28** (10)
Book	– (0)	**46.50 (10)**
EachMovie	– (0)	**1216.89 (8)**
WebKB	– (0)	**575.68 (10)**
Reuters-52	– (0)	**120.58 (10)**
20 NewsGrp.	– (0)	**504.52 (9)**
BBC	– (0)	**2757.18 (3)**
Ad	– (0)	**1254.37 (8)**

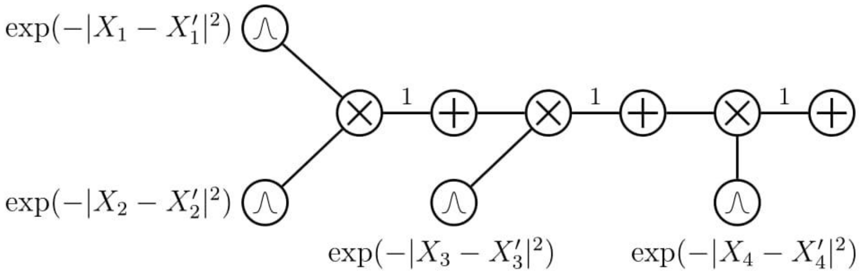
YooJung Choi, Tal Friedman and Guy Van den Broeck. Solving Marginal MAP Exactly by Probabilistic Circuit Transformations, 2021.

Tractable Computation of Expected Kernels

- How to compute the expected kernel given two distributions **p**, **q**?

$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$$

- Circuit representation for kernel functions, e.g., $\mathbf{k}(\mathbf{x},\mathbf{x}') = \exp\left(-\sum_{i=1}^{4} \mid X_i - X_i' \mid^2\right)$



Wenzhe Li, Zhe Zeng, Antonio Vergari and Guy Van den Broeck. Tractable Computation of Expected Kernels, *UAI*, 2021.

Tractable Computation of Expected Kernels: Applications

- Reasoning about support vector regression (SVR) with missing features

$$\mathbb{E}_{\mathbf{x}_m \sim \mathbf{p}(\mathbf{X}_m|\mathbf{x}_o)} \left[\sum_{i=1}^{m} w_i \mathbf{k}(\mathbf{x}_i, \mathbf{x}) + b \right]$$

missing features

SVR model

- Collapsed Black-box Importance Sampling: minimize kernelized Stein discrepancy

importance weights $\boldsymbol{w}^* = \underset{\boldsymbol{w}}{\operatorname{argmin}} \left\{ \boldsymbol{w}^\top \boldsymbol{K}_{p,\mathbf{s}} \boldsymbol{w} \,\middle|\, \sum_{i=1}^{n} w_i = 1,\ w_i \geq 0 \right\}$

expected kernel matrix

Wenzhe Li, Zhe Zeng, Antonio Vergari and Guy Van den Broeck. Tractable Computation of Expected Kernels, *UAI*, 2021.

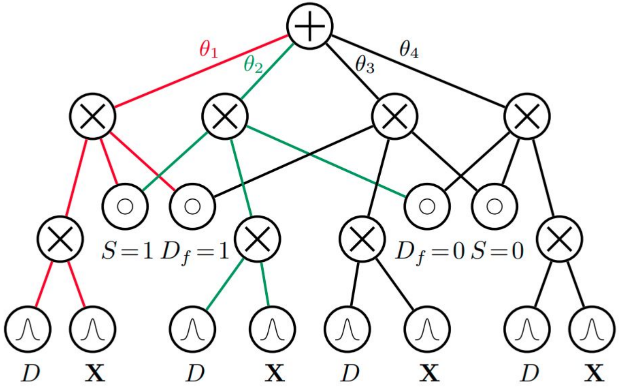
Model-Based Algorithmic Fairness: FairPC

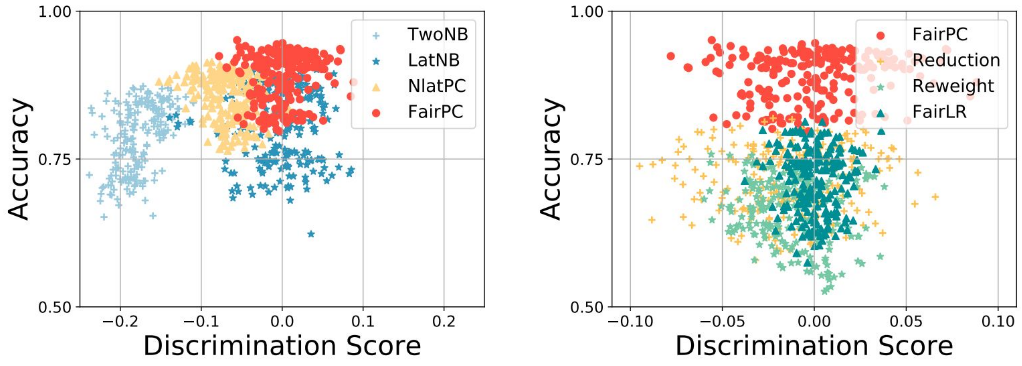
Learn classifier given
- features S and X
- training labels/decisions D

Group fairness by demographic parity:

Fair decision D_f should be independent of the sensitive attribute S

Discover the **latent fair decision** D_f by learning a PC.





[Choi et al. AAAI21]

Probabilistic Sufficient Explanations

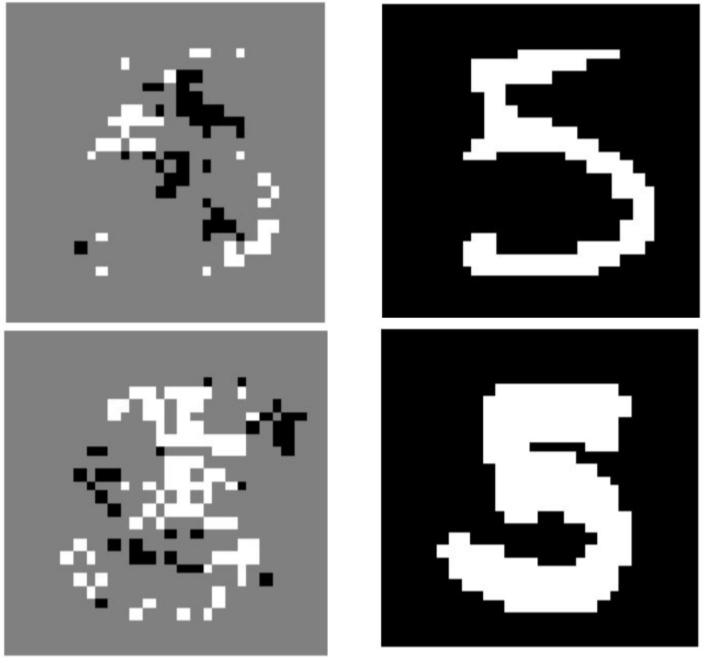
<u>Goal</u>: explain an instance of classification (a specific prediction)

Explanation is a subset of features, s.t.

1. The explanation is "probabilistically sufficient"

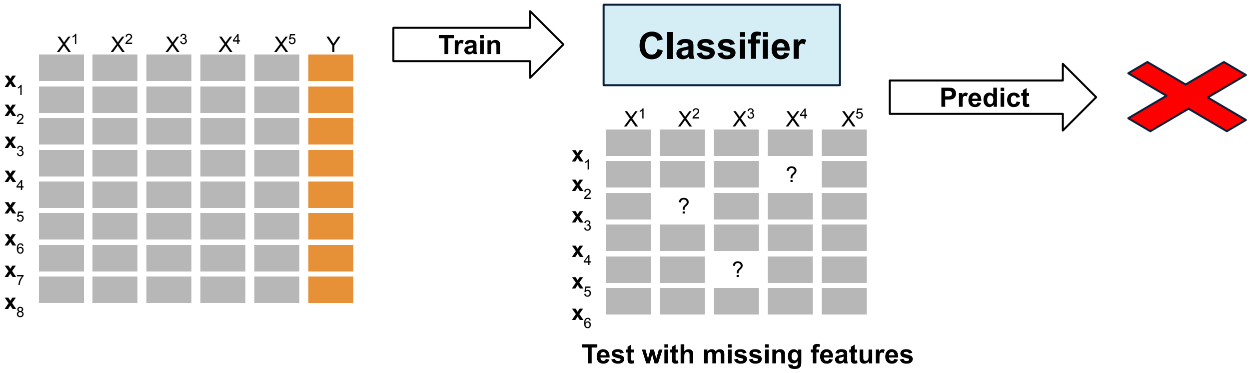
   Under the feature distribution, given the explanation, the classifier is likely to make the observed prediction.

2. It is minimal and "simple"



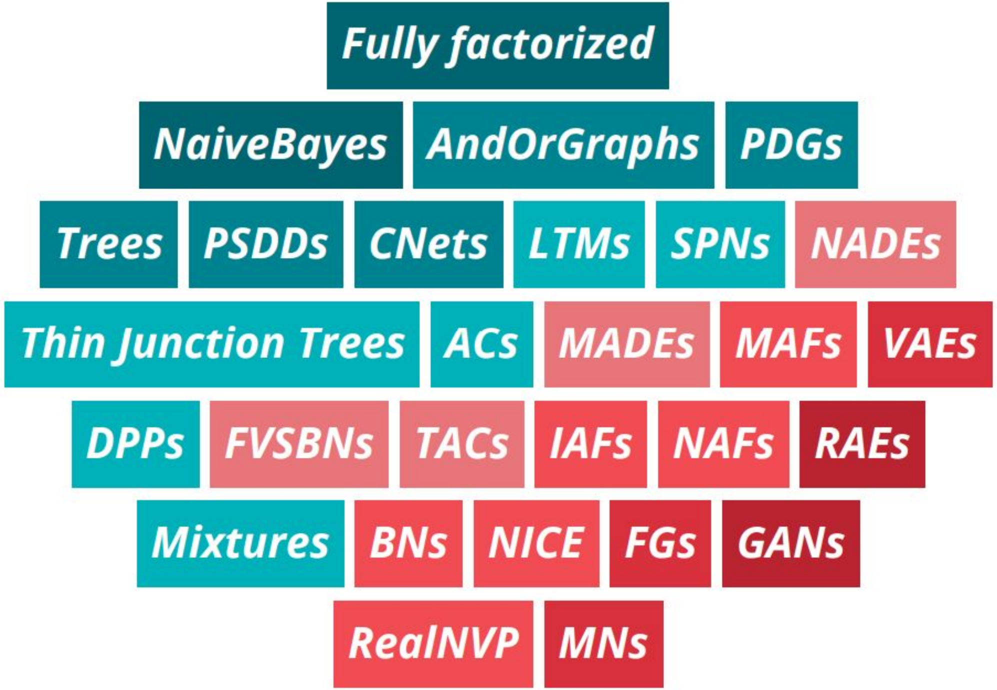
[Khosravi et al. IJCAI19, Wang et al. XXAI20]

Prediction with Missing Features

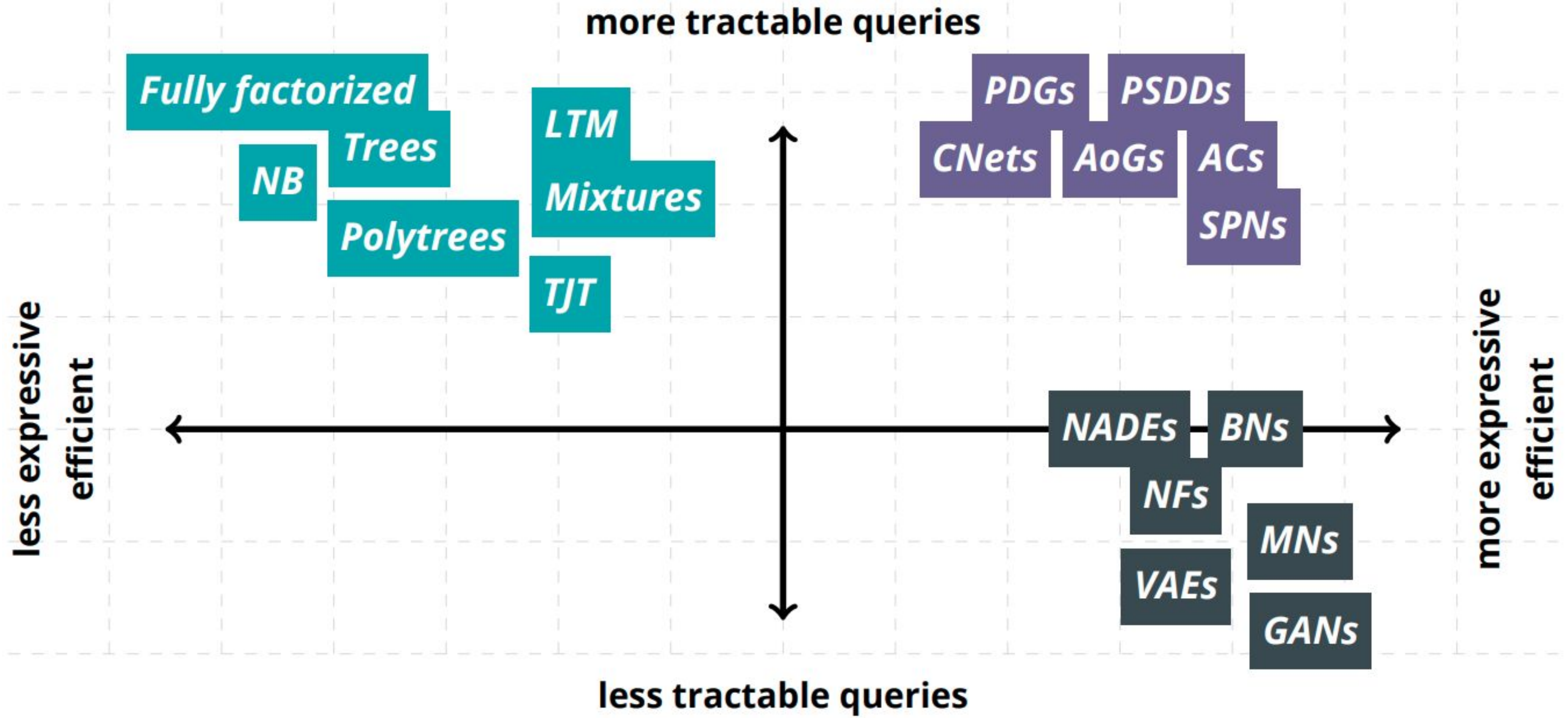


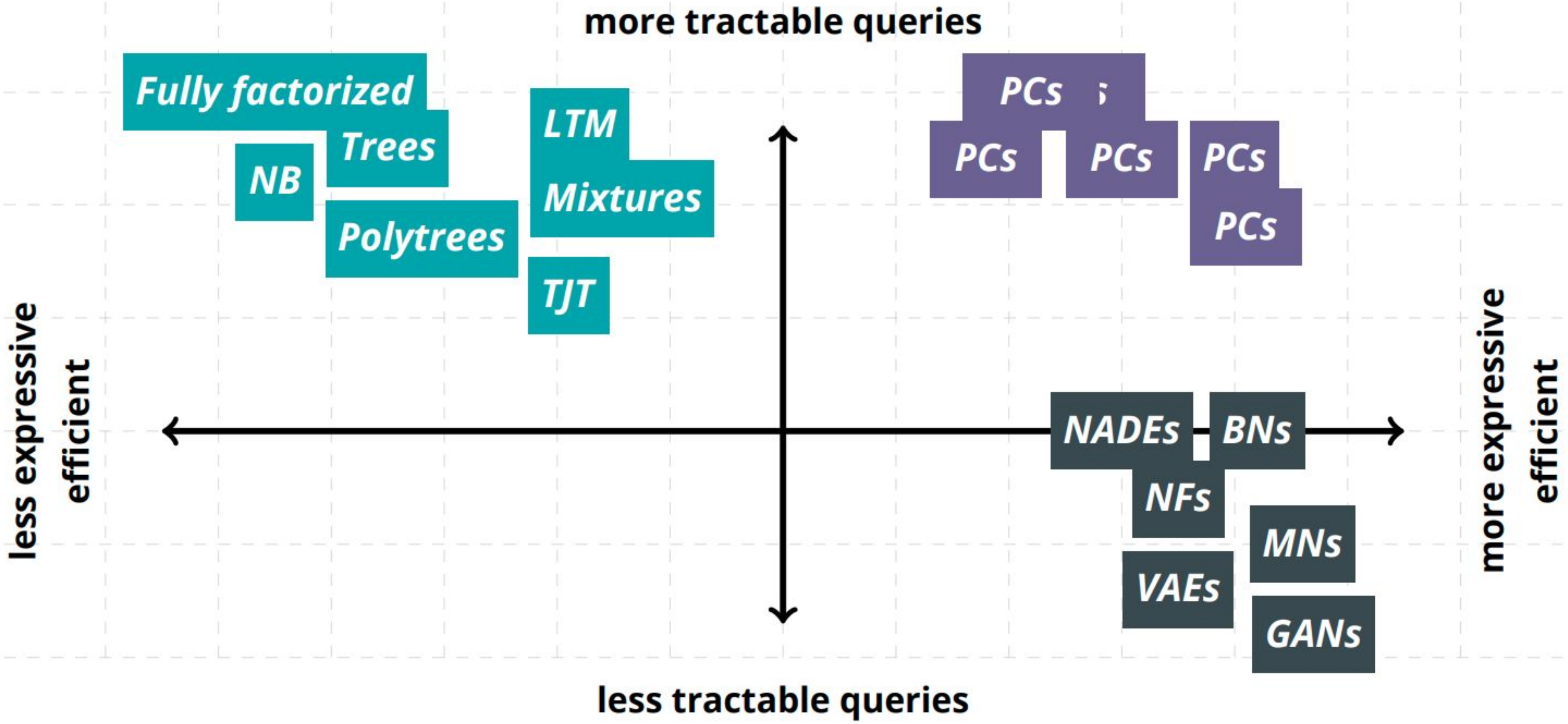
See work on

- Expected predictions / conformant learning [Khosravi et al.]
- Generative forests [Correia et al.]



tractability is a spectrum


more tractable queries
Fully factorized
Trees
NB
Polytrees
LTM
Mixtures
TJT
PDGs
PSDDs
CNets
AoGs
ACs
SPNs
less expressive
efficient
more expressive
efficient
NADEs
BNs
NFs
MNs
VAEs
GANs
less tractable queries


more tractable queries
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Trees
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TJT
PCs
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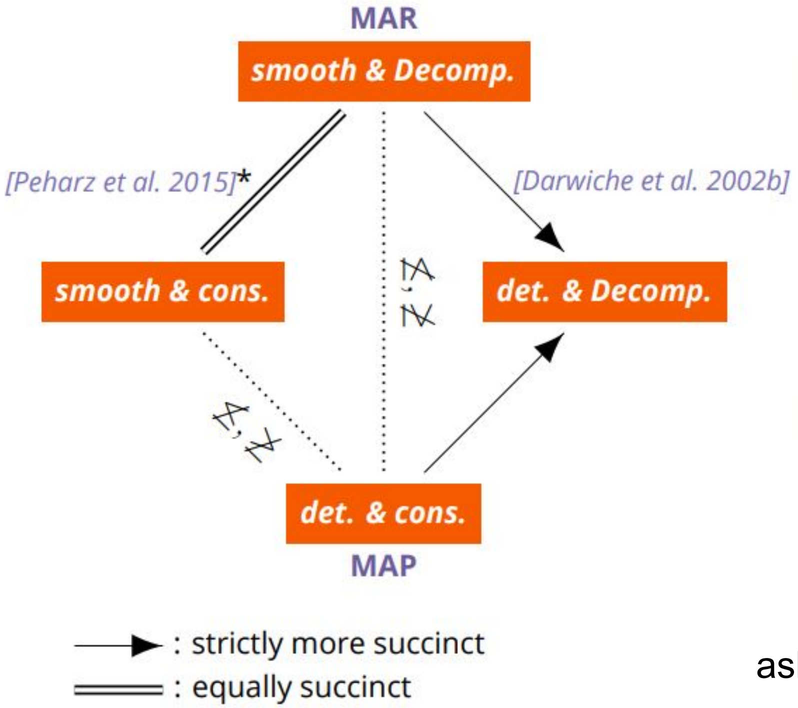
GANs
less tractable queries

Outline

1. What are tractable probabilistic circuits?
2. Are these models any good?
3. How far can we push tractable inference?
4. **What is their expressive power?**

Expressive efficiency of circuits



- 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"*

ask YooJung Choi and Stefan Mengel

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

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

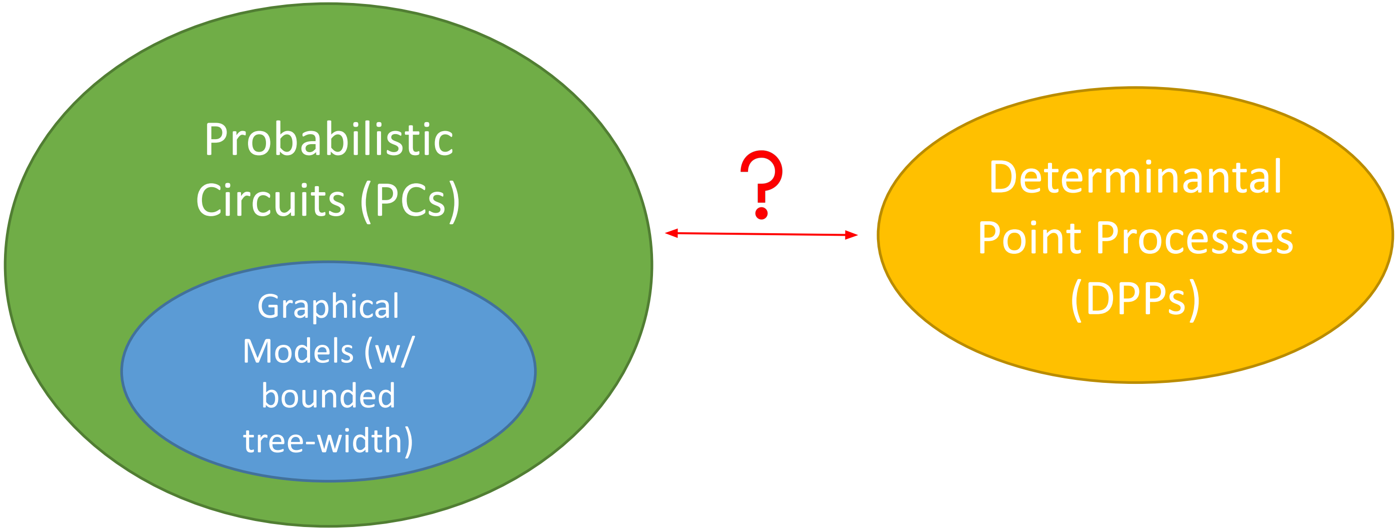
Tractable likelihoods and marginals

Global Negative Dependence

Diversity in recommendation systems

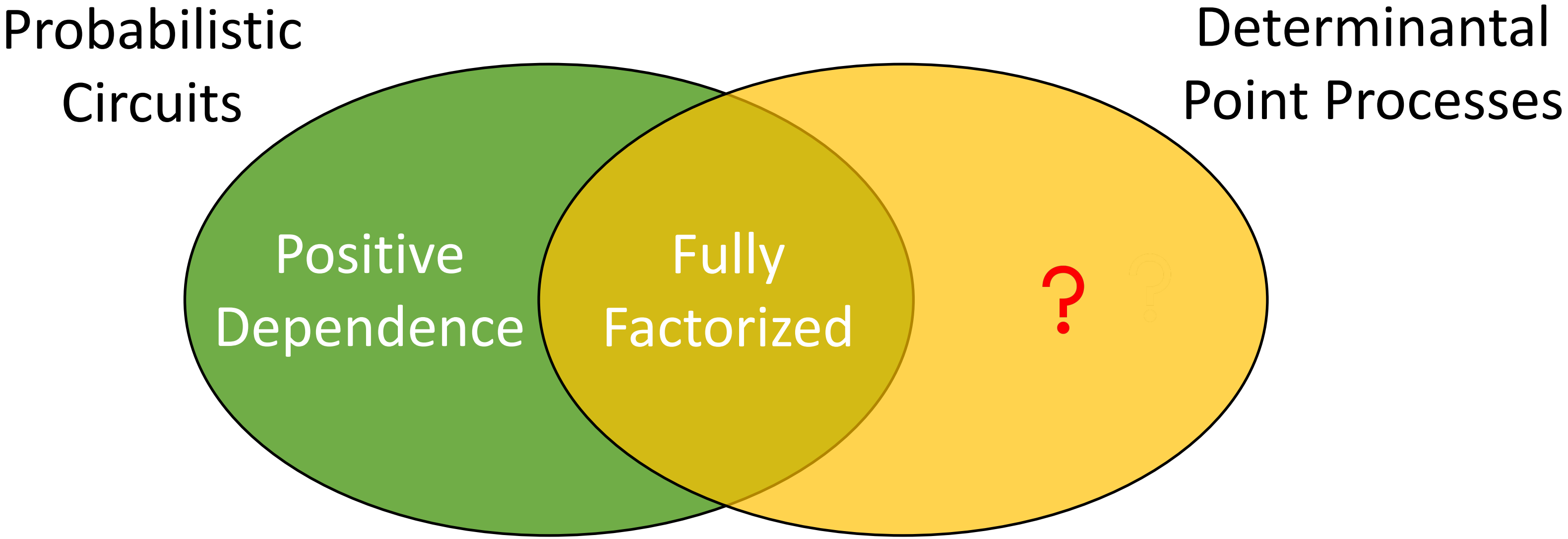
$$\Pr_L(X_1 = 1, X_2 = 0, X_3 = 1, X_4 = 0) = \frac{1}{\det(L + I)} \det(L_{\{1,2\}})$$

Are all tractable probabilistic models probabilistic circuits?



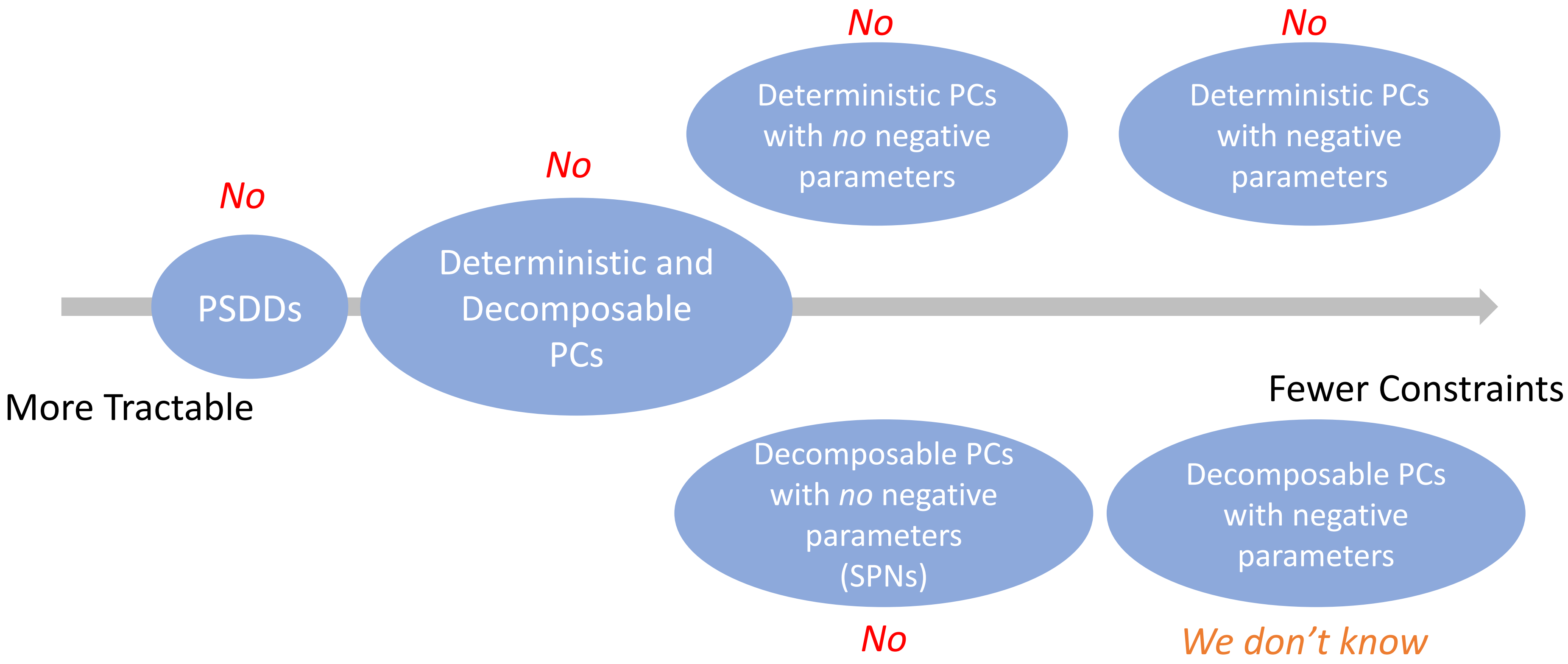
Honghua Zhang, Steven Holtzen and Guy Van den Broeck. On the Relationship Between Probabilistic Circuits and Determinantal Point Processes, *UAI*, 2020.

Relationship between PCs and DPPs



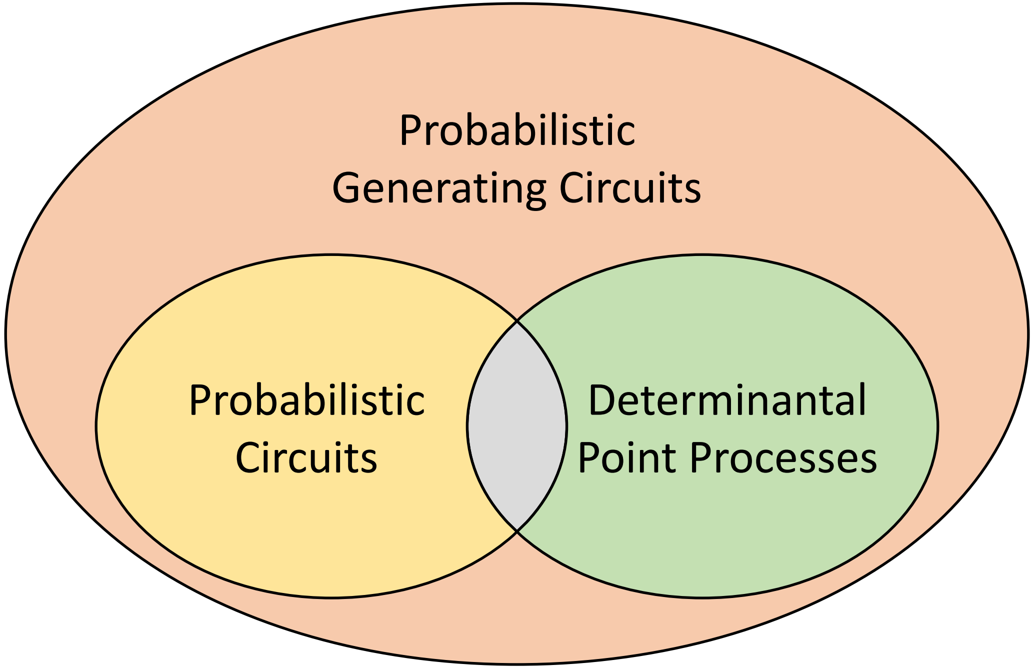
Honghua Zhang, Steven Holtzen and Guy Van den Broeck. On the Relationship Between Probabilistic Circuits and Determinantal Point Processes, *UAI*, 2020.

We cannot tractably represent DPPs with subclasses of PCs



Honghua Zhang, Steven Holtzen and Guy Van den Broeck. On the Relationship Between Probabilistic Circuits and Determinantal Point Processes, *UAI*, 2020.

Probabilistic Generating Circuits



A Tractable Unifying Framework for PCs and DPPs

Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

Probability Generating Functions

X_1	X_2	X_3	$\Pr_\beta$
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

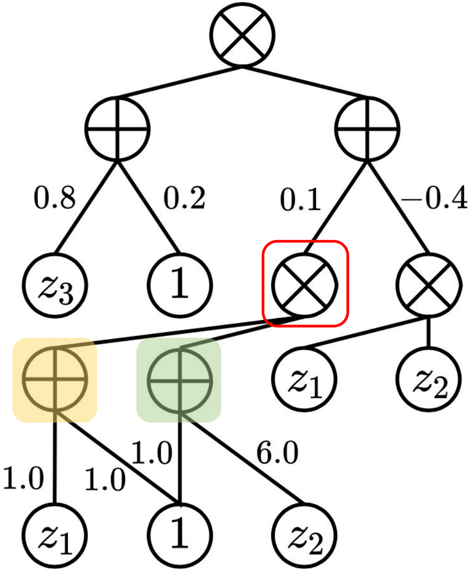
$$g_\beta = 0.16 z_1 z_2 z_3 + 0.04 z_1 z_2 + 0.08 z_1 z_3 + 0.02 z_1 + 0.48 z_2 z_3 + 0.12 z_2 + 0.08 z_3 + 0.02.$$

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

Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

Probabilistic Generating Circuits (PGCs)

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



1. Sum nodes ⊕ with weighted edges to children.
2. Product nodes ⊗ with unweighted edges to children.
3. Leaf nodes: z_i or constant.

Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

DPPs as PGCs

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

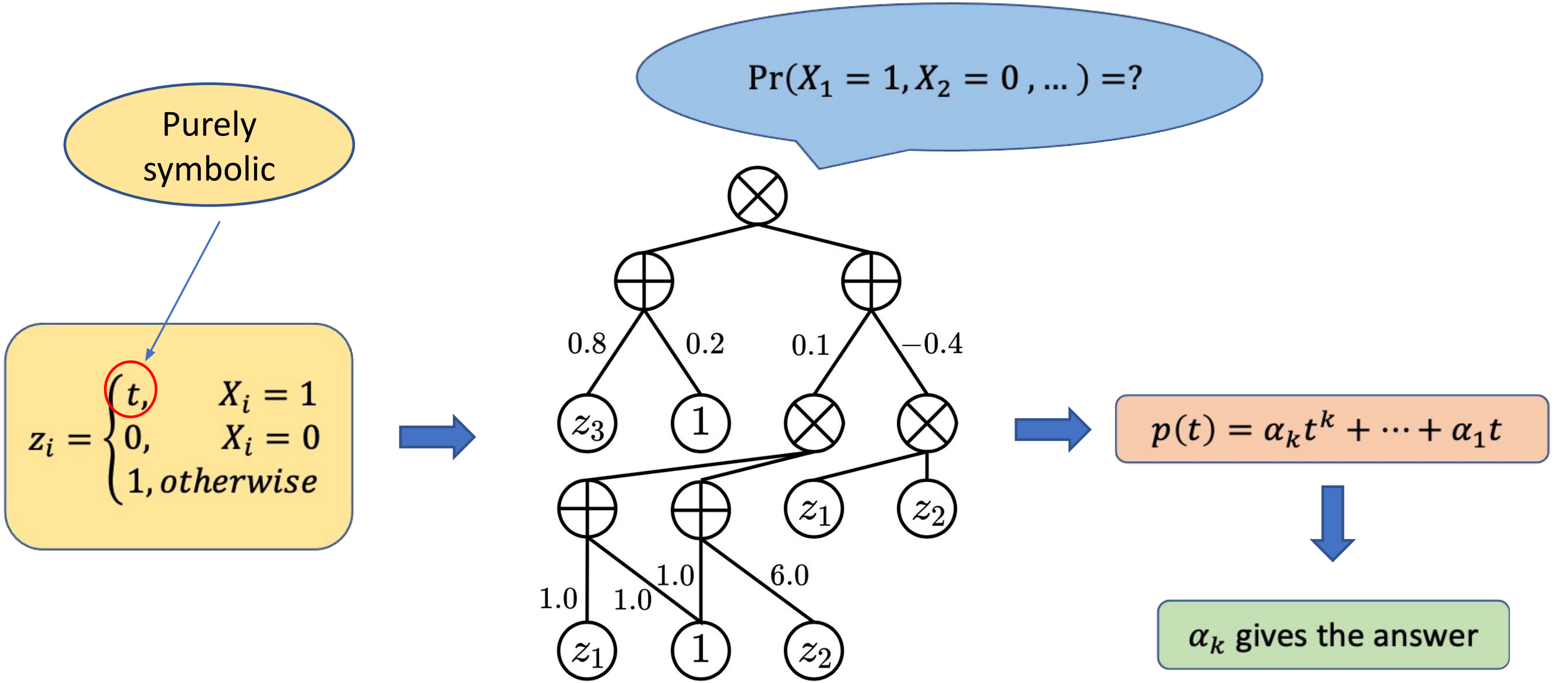
$$g_L = \frac{1}{\det(L+I)} \det(I + L\mathrm{diag}(z_1, \dots, z_n)).$$

Constant

Division-free determinant algorithm
(Samuelson-Berkowitz algorithm)

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

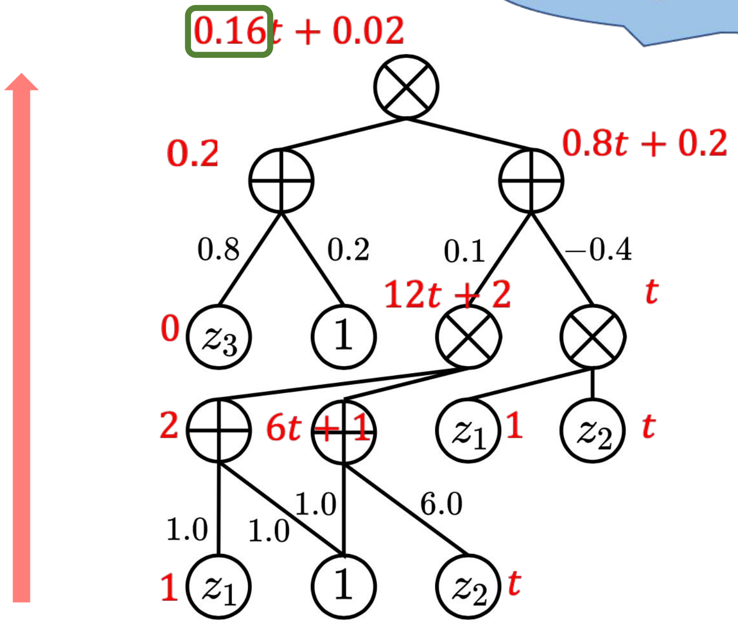
PGCs Support Tractable Likelihoods/Marginals



Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

Example

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



X_1	X_2	X_3	$\Pr_\beta$
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Experiment Results: Amazon Baby Registries

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

SimplePGC achieves SOTA result on 11/15 datasets

Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

Conclusion

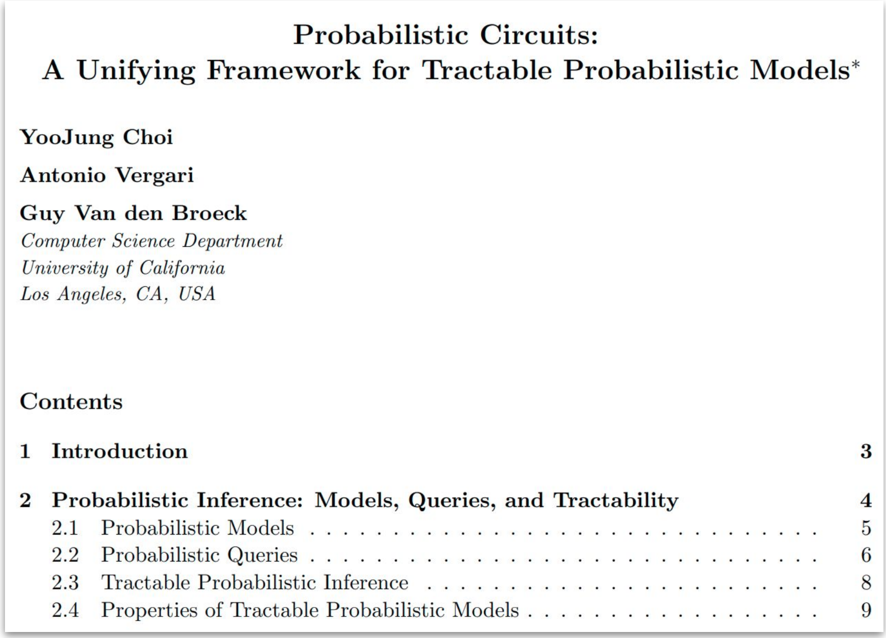
1. What are tractable probabilistic circuits?
2. Are these models any good?
3. How far can we push tractable inference?
4. What is their expressive power?

Learn more about probabilistic circuits?

Tutorial (3h)

https://youtu.be/2RAG5-L9R70

Overview Paper (80p)



Probabilistic Circuits:
A Unifying Framework for Tractable Probabilistic Models*

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Contents

http://starai.cs.ucla.edu/papers/ProbCirc20.pdf