UCLA Computer Science

STAR AI RESEARCH LAB UCLA

Tractable Probabilistic Circuits

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Simons Institute - Algorithmic Aspects of Causal Inference - Mar 20, 2022

Outline

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

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

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

Fully factorized

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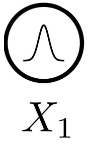
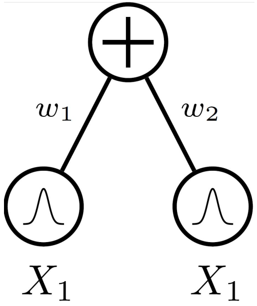
RealNVP MNs

a *unifying framework* for tractable models

Probabilistic circuits

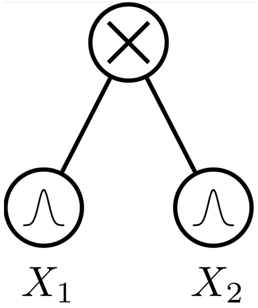
computational graphs that recursively define distributions





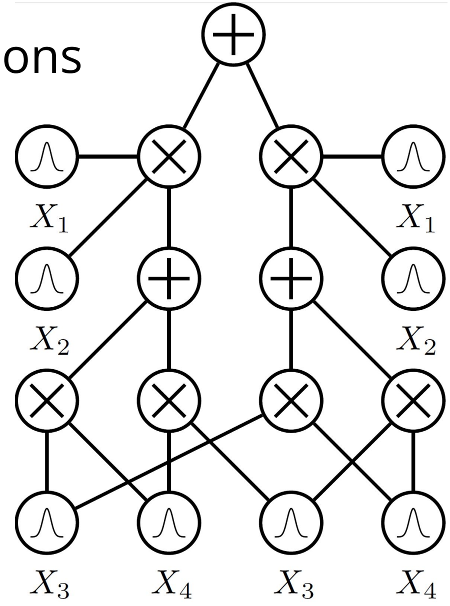
$$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$$

⇒ *mixtures*



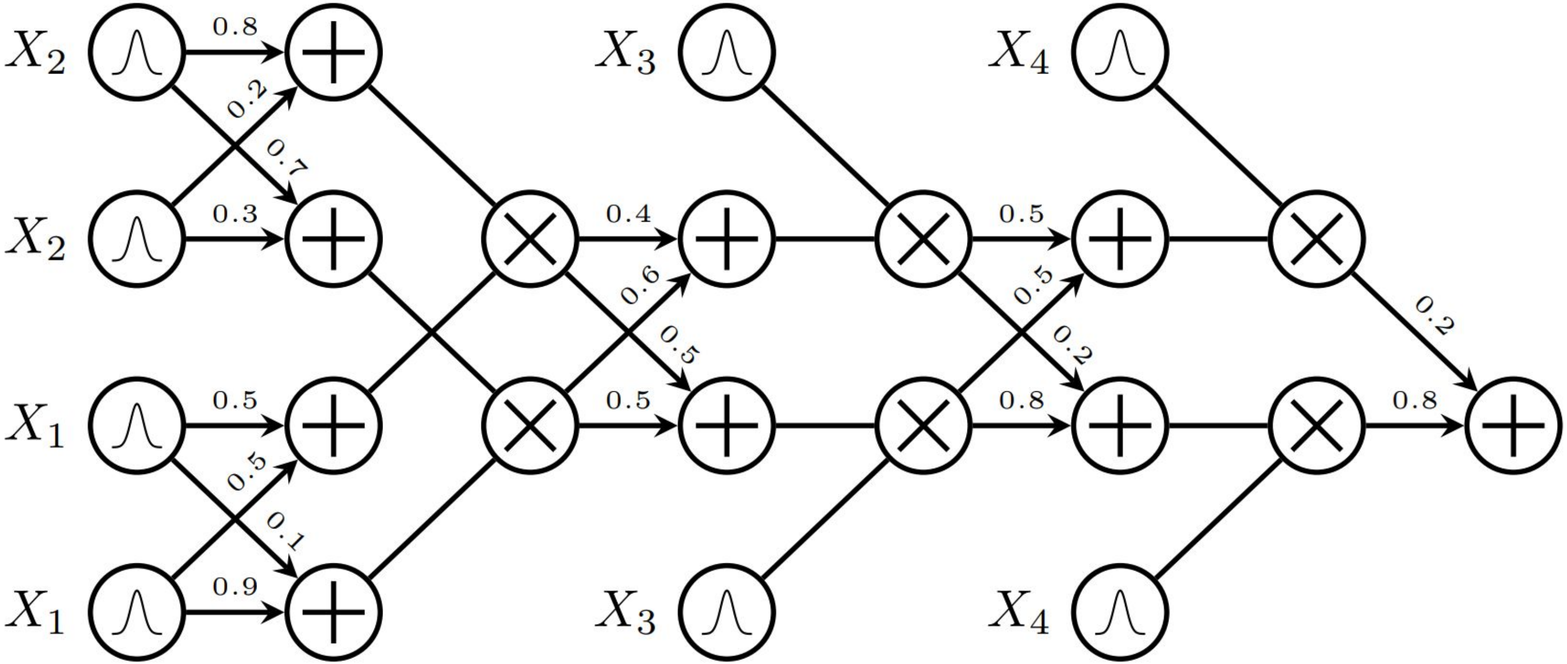
$$p(X_1, X_2) = p(X_1) \cdot p(X_2)$$

⇒ *factorizations*



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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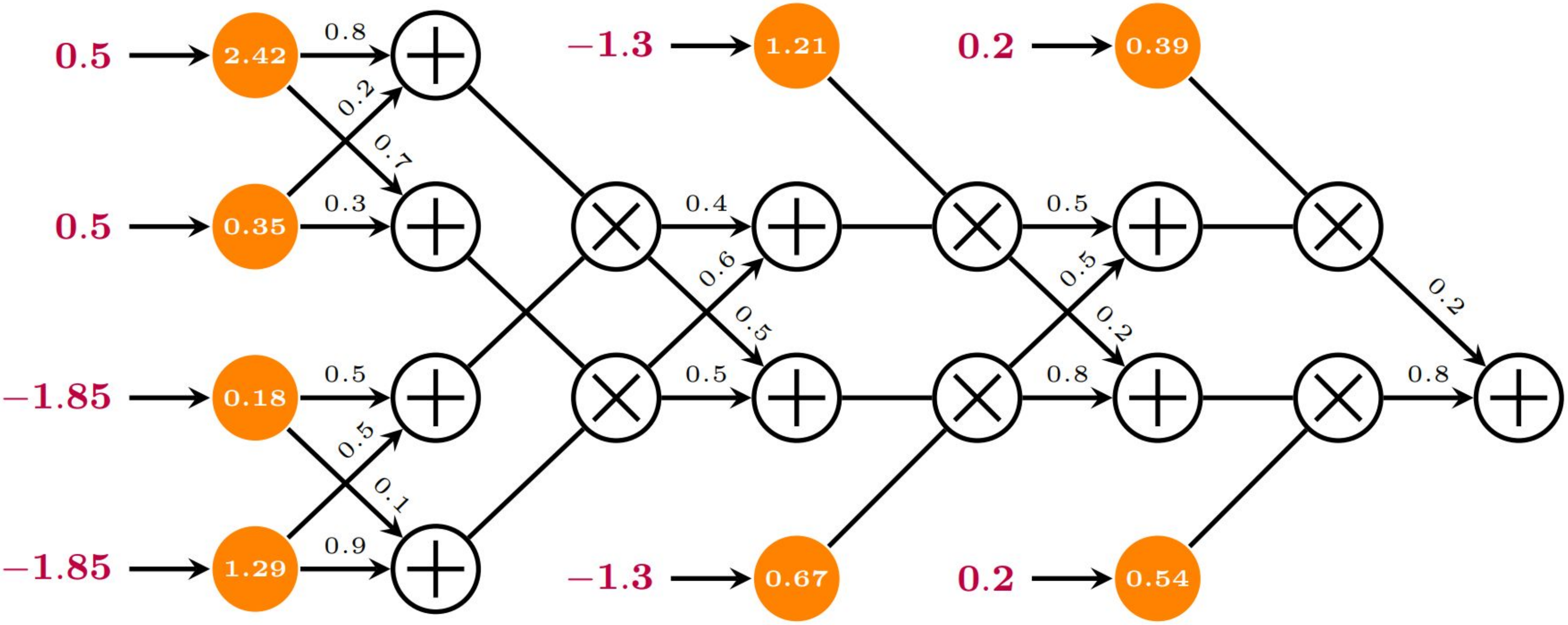

Likelihood

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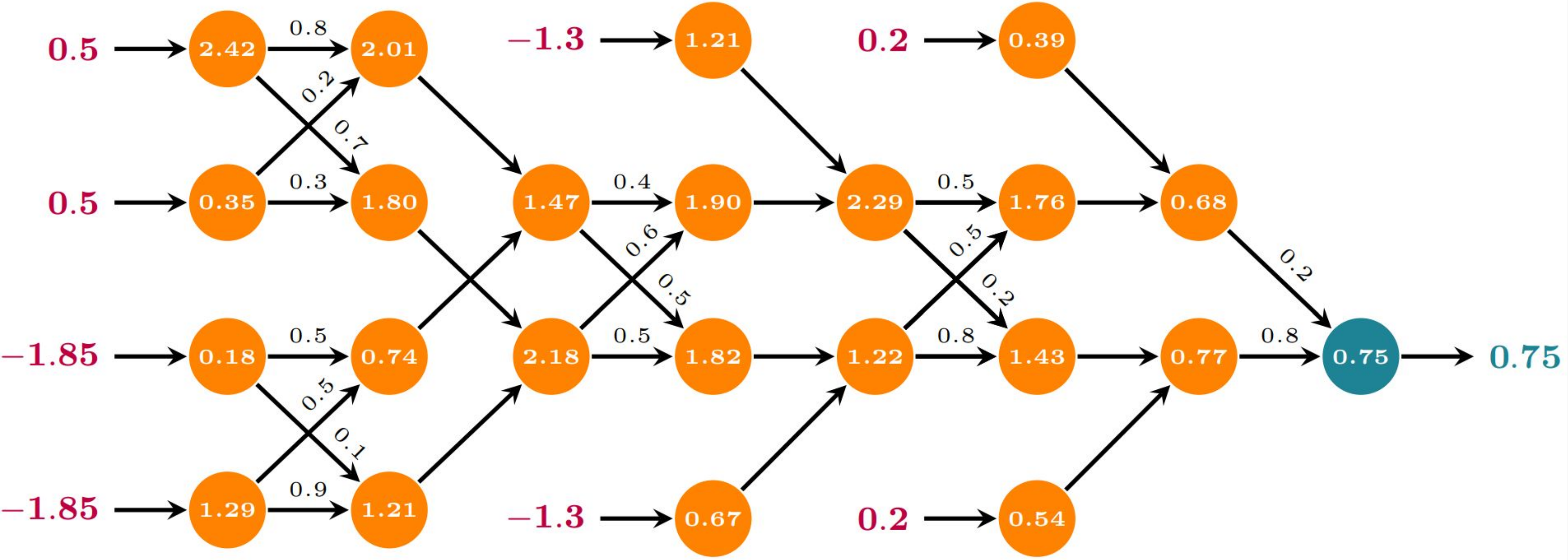
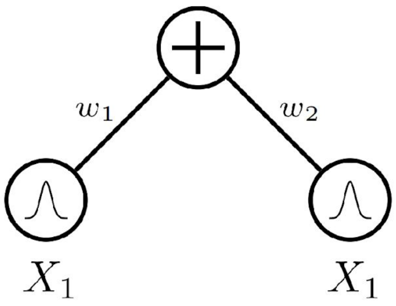


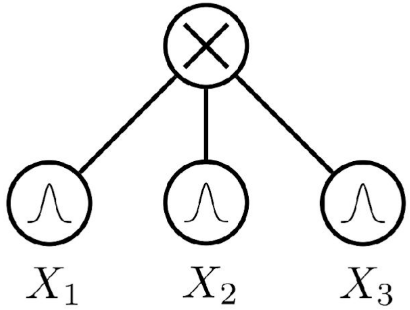
Tractable marginals

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

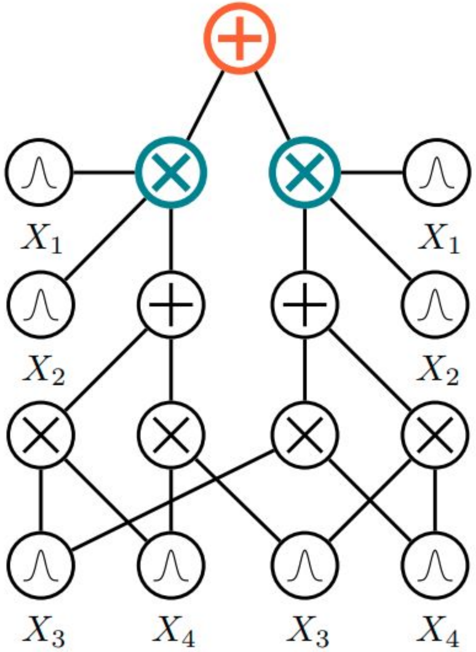
Smoothness + decomposability = tractable MAR

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**

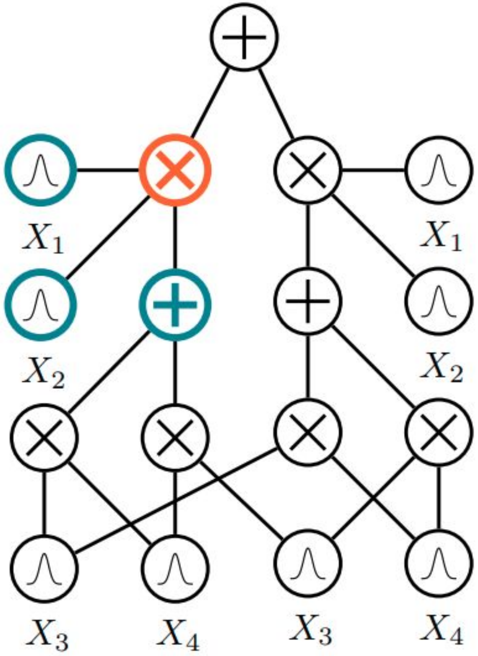
If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (***decomposability***):

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

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

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

$\Rightarrow$ *integrals decompose into easier ones*



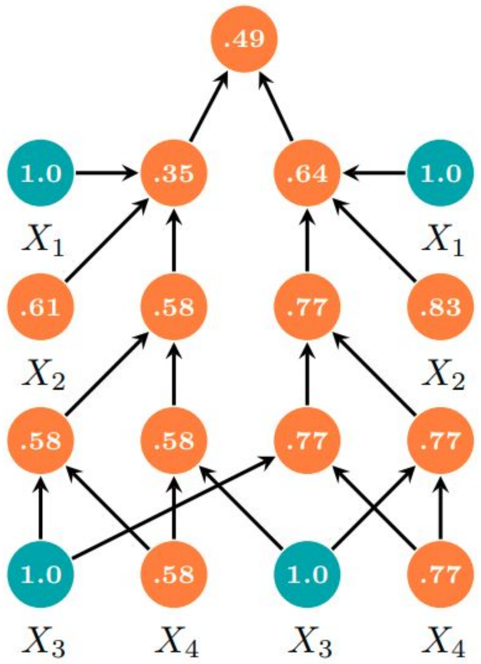
Smoothness + decomposability = tractable MAR

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 $\boldsymbol{Z}_i = \int p(x_i)dx_i$
  - $\Rightarrow$ *for normalized leaf distributions:* 1.0
- leafs over X_2 and X_4 output ***EVI***
- feedforward evaluation (bottom-up)



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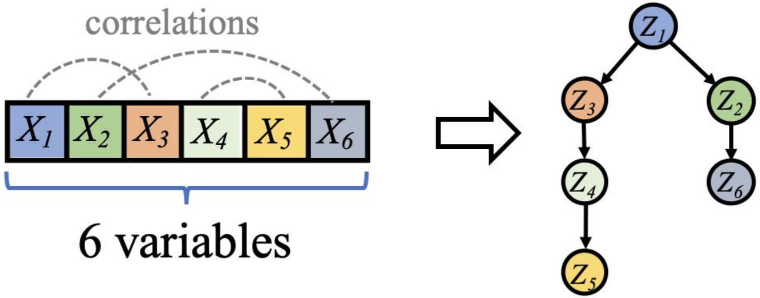
Learning Expressive Probabilistic Circuits

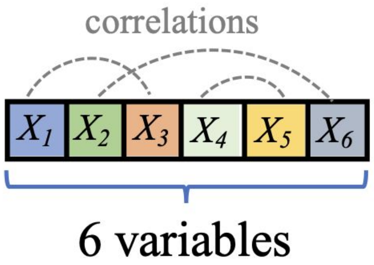
Hidden Chow-Liu Trees

Learned **CLT structure** captures strong pairwise dependencies

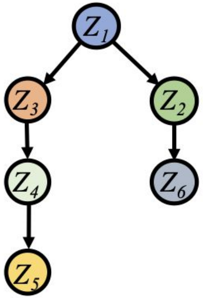


Learning Expressive Probabilistic Circuits

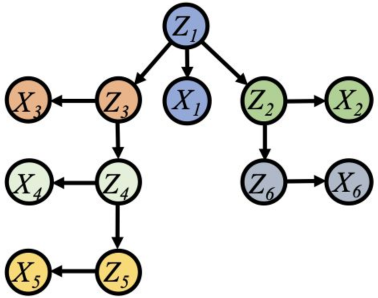
Hidden Chow-Liu Trees



Learned **CLT structure** captures strong pairwise dependencies



Learned **HCLT structure**

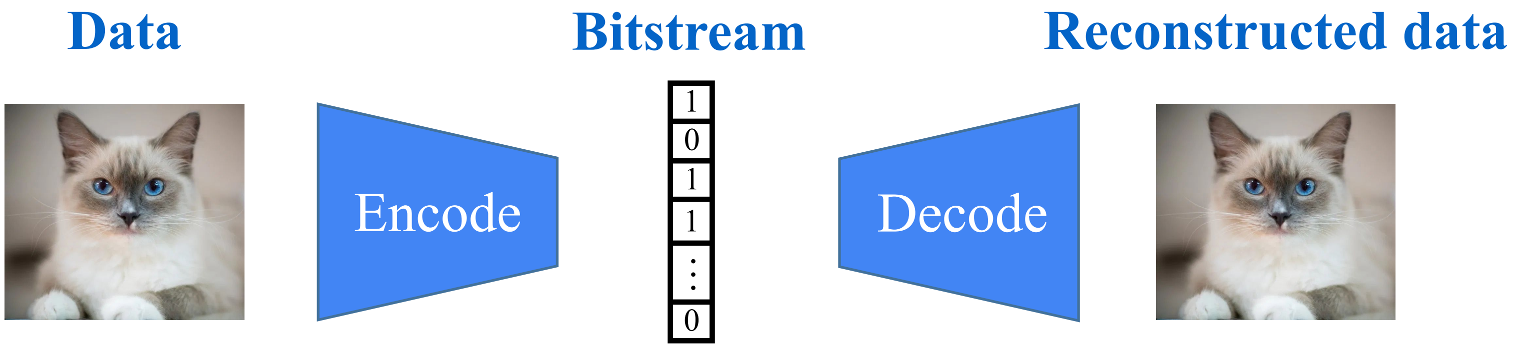


Compile into an equivalent PC

Mini-batch Stochastic **Expectation Maximization**

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

Lossless 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.

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Expressive models without *compromises*

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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

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

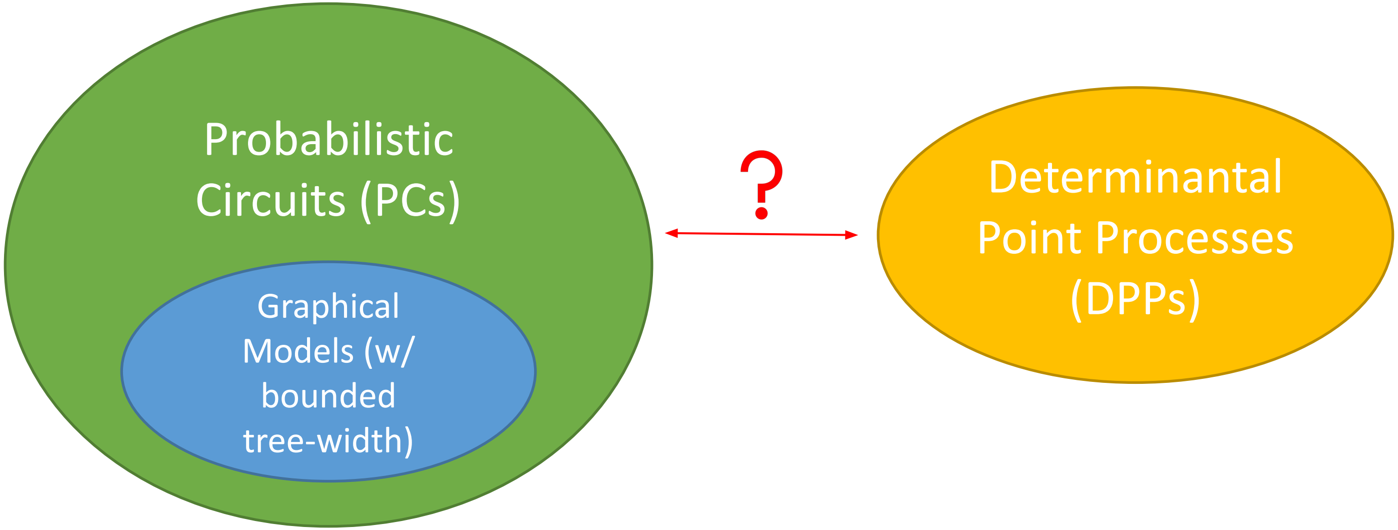
Tractable likelihoods and marginals

Global Negative Dependence

Diversity in recommendation systems

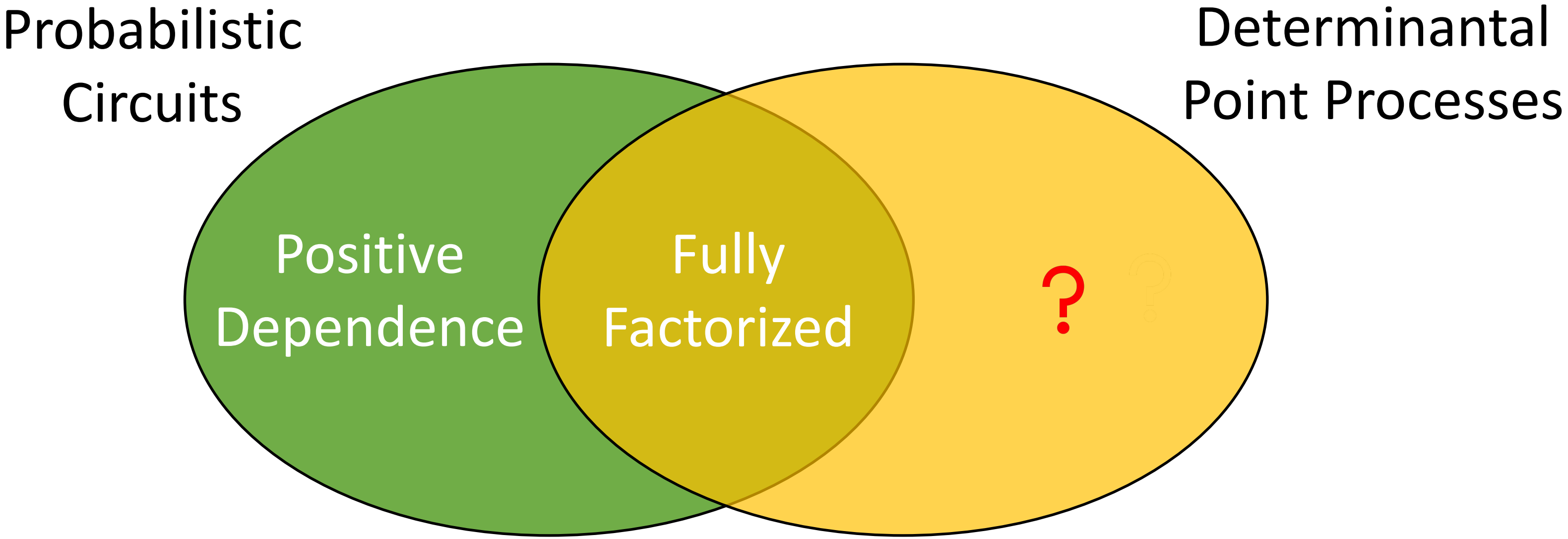
$$\Pr_L(X_1 = 1, X_2 = 0, X_3 = 1, X_4 = 0) = \frac{1}{\det(L + I)} \det(L_{\{1,2\}})$$

Are all tractable probabilistic models probabilistic circuits?



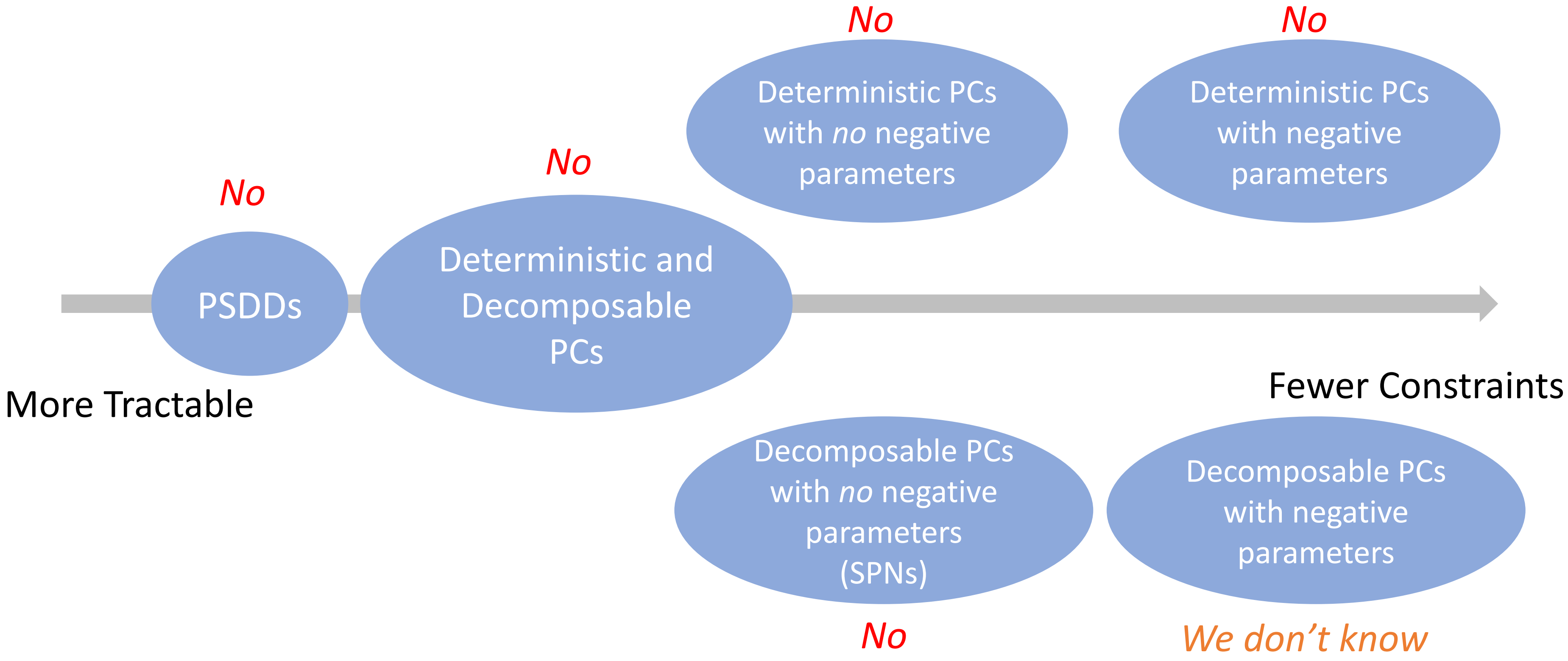
Honghua Zhang, Steven Holtzen and Guy Van den Broeck. On the Relationship Between Probabilistic Circuits and Determinantal Point Processes, *UAI*, 2020.

Relationship between PCs and DPPs



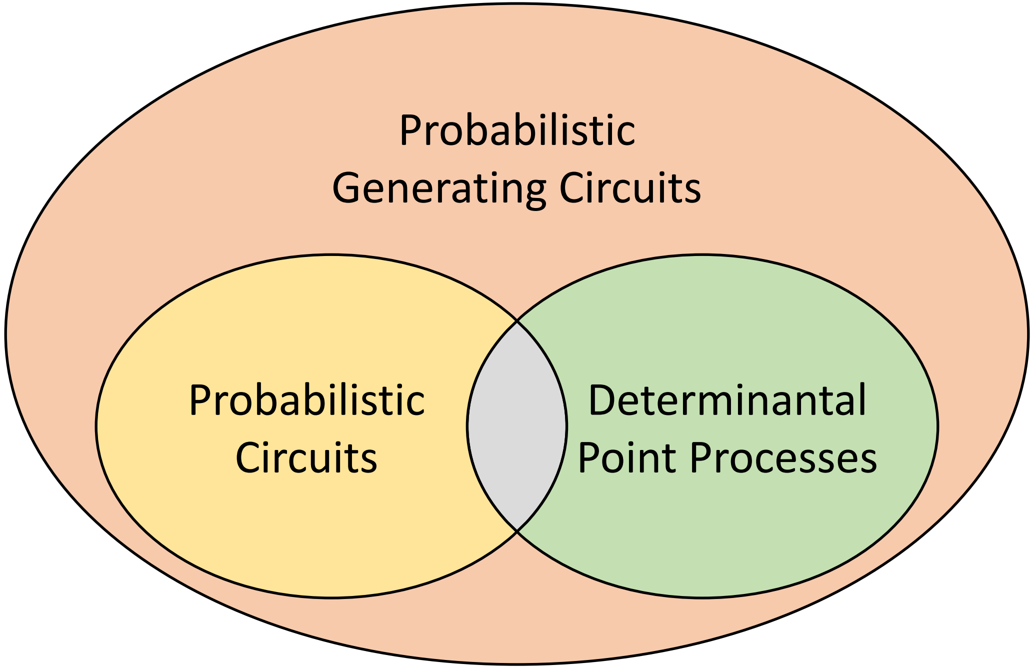
Honghua Zhang, Steven Holtzen and Guy Van den Broeck. On the Relationship Between Probabilistic Circuits and Determinantal Point Processes, *UAI*, 2020.

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

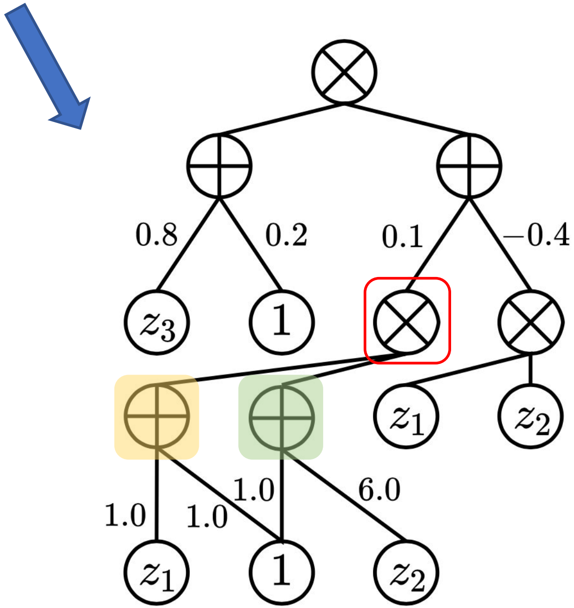
$$g_\beta = 0.16 z_1 z_2 z_3 + 0.04 z_1 z_2 + 0.08 z_1 z_3 + 0.02 z_1 + 0.48 z_2 z_3 + 0.12 z_2 + 0.08 z_3 + 0.02.$$

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

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

Probabilistic Generating Circuits (PGCs)

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



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.

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:

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

Constant

Division-free determinant algorithm
(Samuelson-Berkowitz algorithm)

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

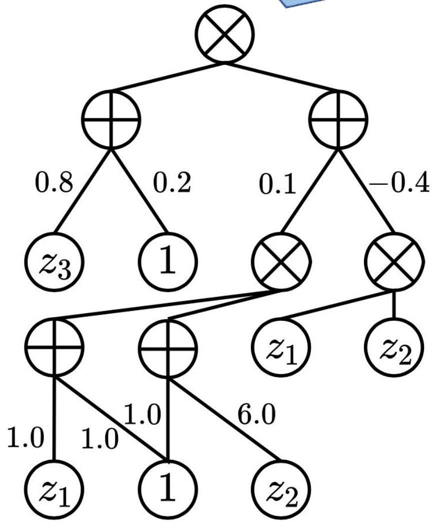
Honghua Zhang, Brendan Juba and Guy Van den Broeck. Probabilistic Generating Circuits, *ICML*, 2021.

PGCs Support Tractable Likelihoods/Marginals

Purely symbolic

$$z_i = \begin{cases} t, & X_i = 1 \\ 0, & X_i = 0 \\ 1, & otherwise \end{cases}$$

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



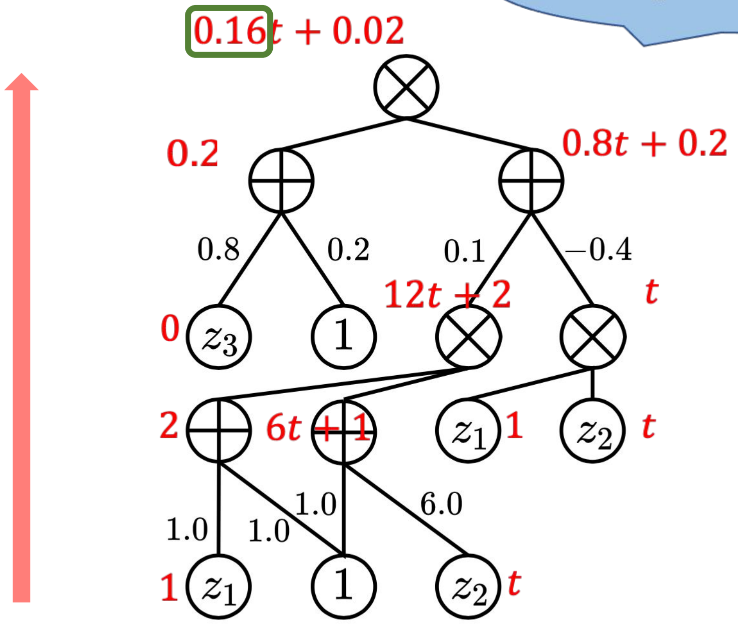
$p(t) = \alpha_k t^k + \cdots + \alpha_1 t$

α_k gives the answer

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	$\Pr_\beta$
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

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

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.

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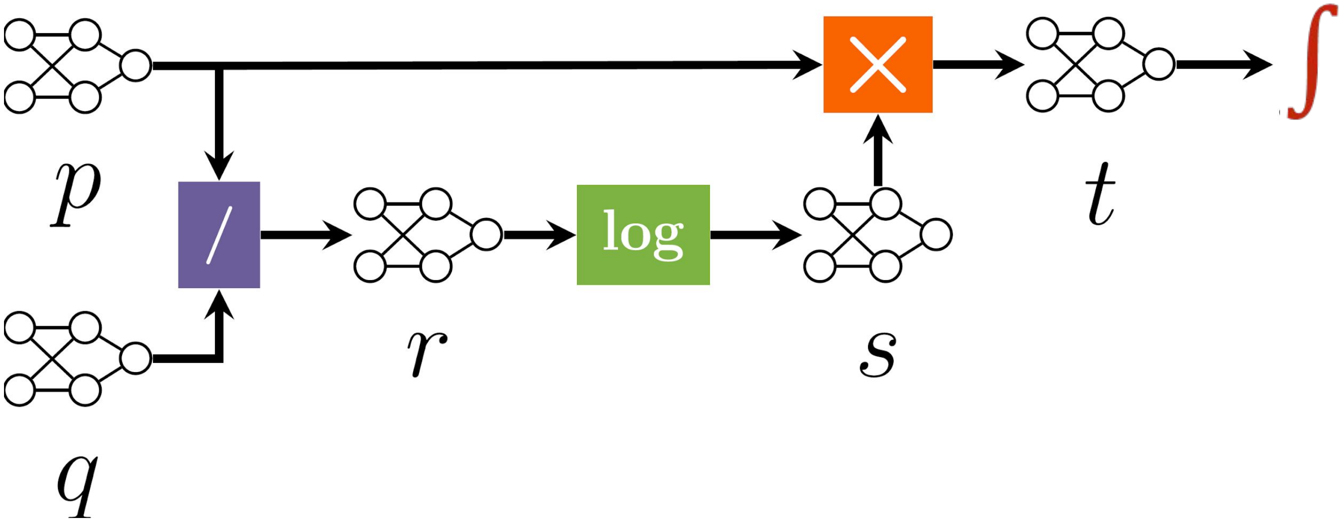
Queries as pipelines: KLD

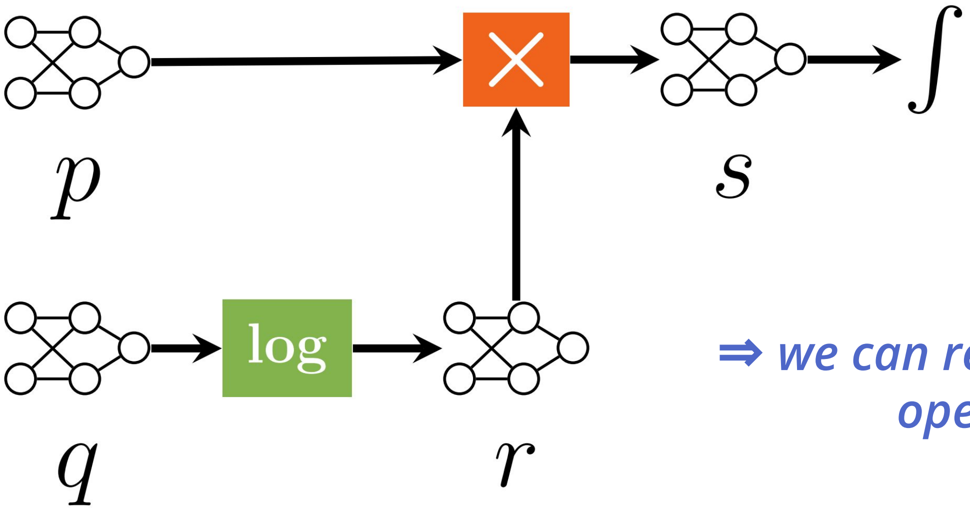
$$\mathbb{KLD}(p \parallel q) = \int p(\boldsymbol{x}) \times \log((p(\boldsymbol{x})/q(\boldsymbol{x}))d\boldsymbol{X}$$



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 $\boldsymbol{e}$,

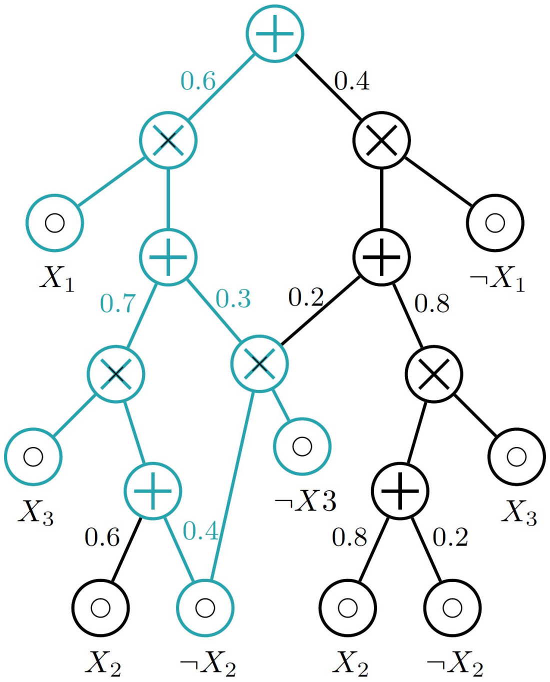
find: $argmax_{\boldsymbol{q}}\, p(\boldsymbol{q}|\boldsymbol{e})$

⇒ *i.e. MAP of a marginal distribution on* $\boldsymbol{Q}$

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

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

Pruning circuits



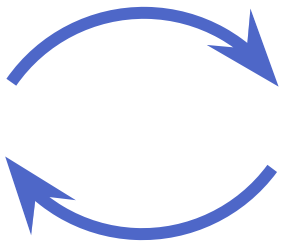
Any parts of circuit not relevant for MMAP state can be pruned away

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)**

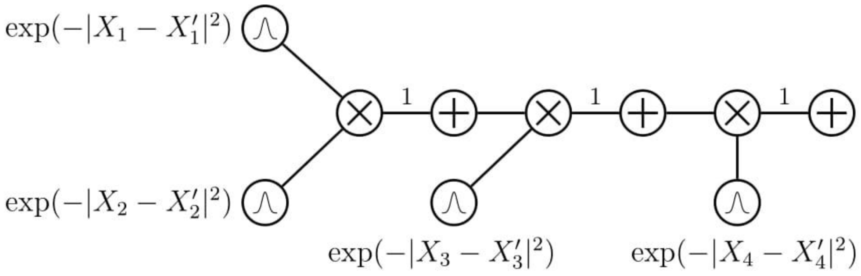
YooJung Choi, Tal Friedman and Guy Van den Broeck. Solving Marginal MAP Exactly by Probabilistic Circuit Transformations, 2021.

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

expected kernel matrix

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

Conclusion

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

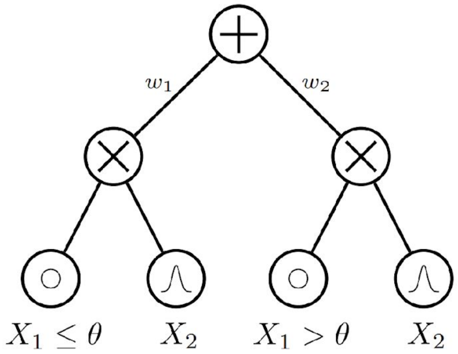
Thanks

This was the work of many wonderful students/postdoc/collaborators!

References: http://starai.cs.ucla.edu/publications/

Determinism

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



deterministic circuit

⇒ *allows **tractable MAP** inference*

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

Darwiche and Marquis, "A Knowledge Compilation Map", 2002