UCLA Computer Science

STAR AI RESEARCH LAB UCLA

Tractable Probabilistic Circuits

Guy Van den Broeck

Beyond Bayes: Paths Towards Universal Reasoning Systems - Jul 21, 2022

Fully factorized

NaiveBayes *AndOrGraphs* *PDGs*

Trees *PSDDs* *CNets* *LTMs* *SPNs* *NADEs*

Thin Junction Trees *ACs* *MADEs* *MAFs* *VAEs*

DPPs *FVSBNs* *TACs* *IAFs* *NAFs* *RAEs*

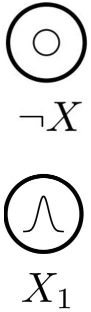
Mixtures *BNs* *NICE* *FGs* *GANs*

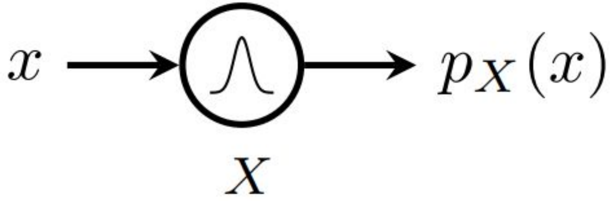
RealNVP *MNs*

a ***unifying framework*** for tractable models

Probabilistic circuits

computational graphs that recursively define distributions



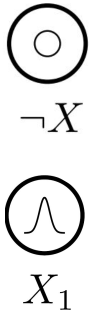


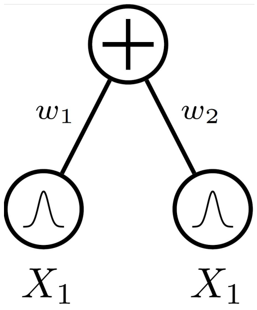
Simple distributions are tractable "black boxes" for:

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

Probabilistic circuits

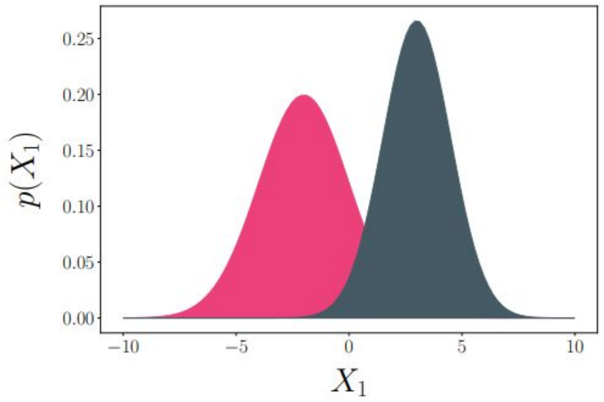
computational graphs that recursively define distributions





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

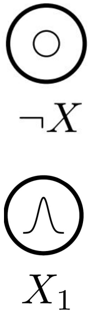
⇒ *mixtures*

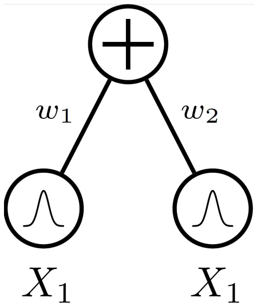


$$p(X) = p(Z = 1) \cdot p_1(X|Z = 1) + p(Z = 2) \cdot p_2(X|Z = 2)$$

Probabilistic circuits

computational graphs that recursively define distributions





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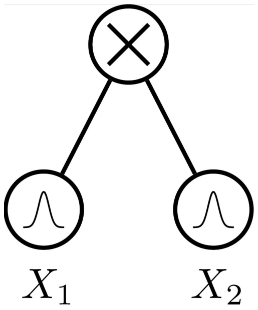
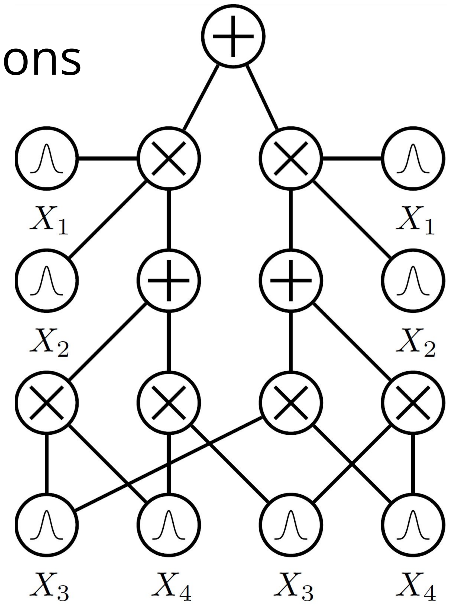
⇒ *mixtures*



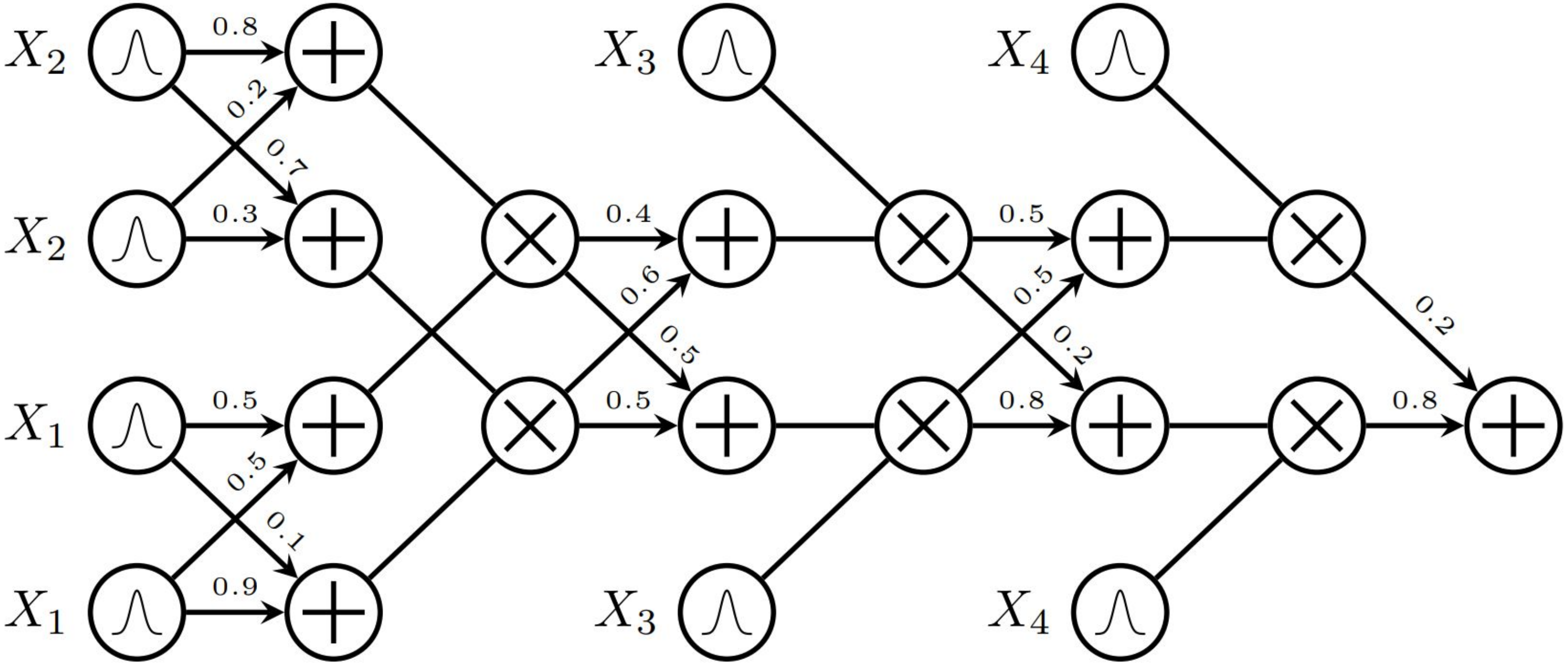
$$p(X_1, X_2) = p(X_1) \cdot p(X_2)$$

⇒ *factorizations*



Likelihood

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



Likelihood

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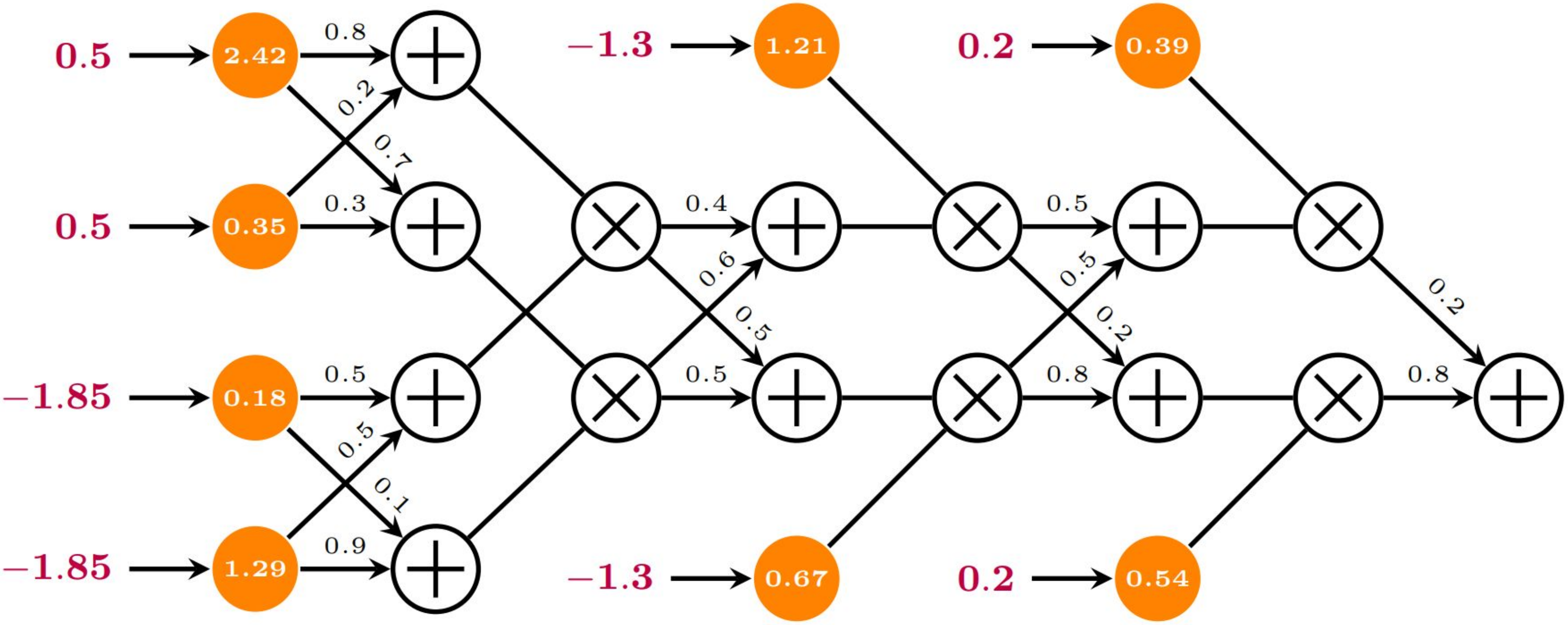

Likelihood

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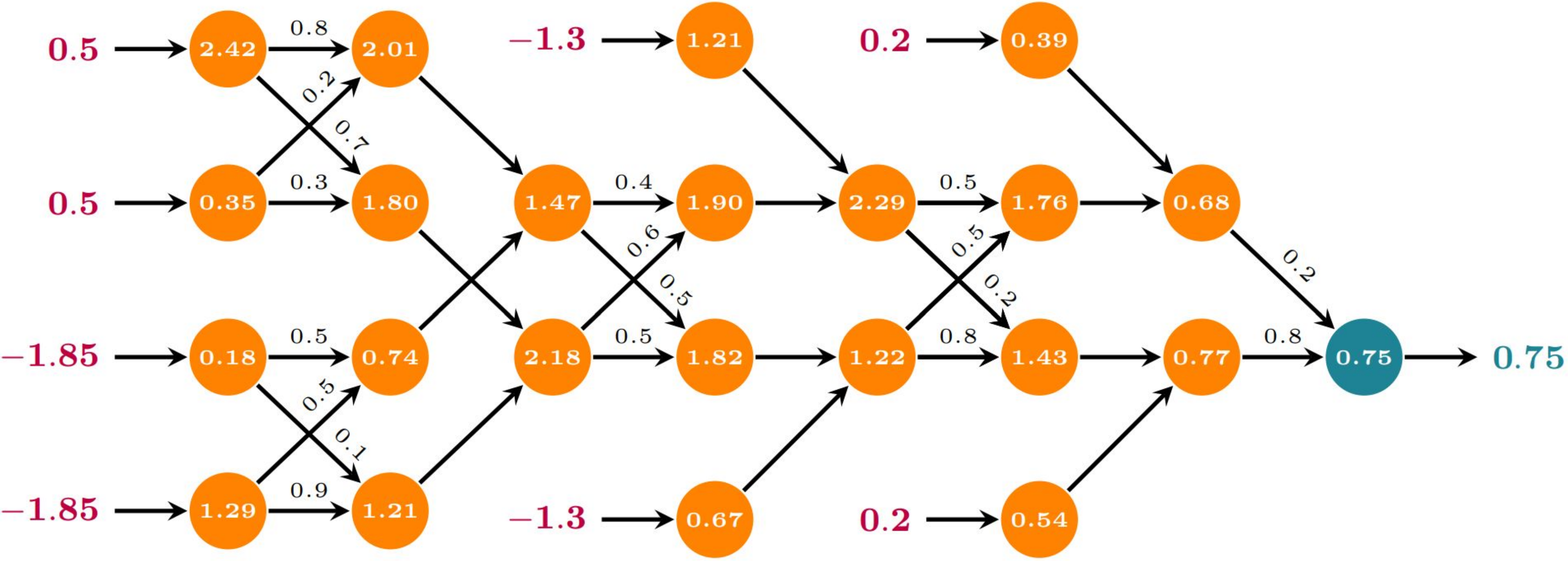
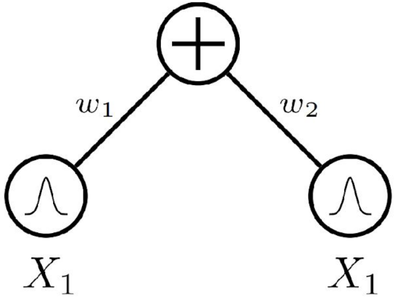


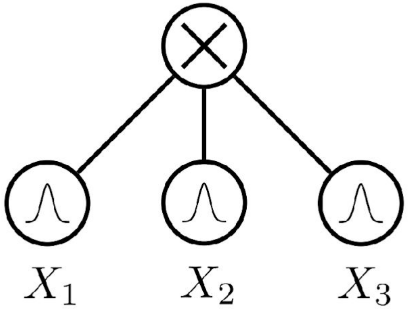
Tractable marginals

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

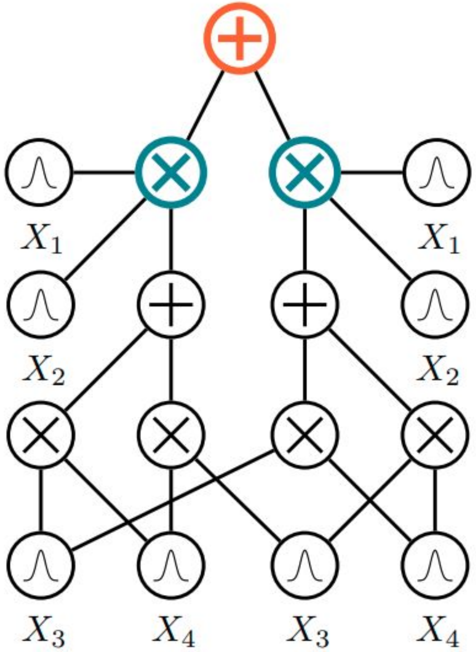
Smoothness + decomposability = tractable MAR

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

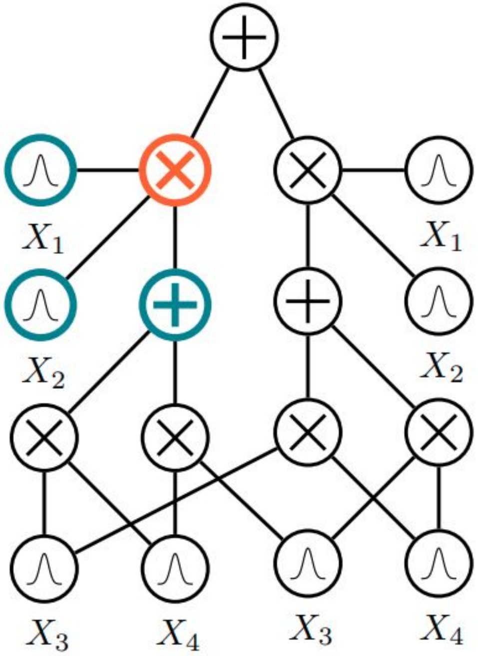
If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (***decomposability***):

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

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

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

$\Longrightarrow$ *integrals decompose into easier ones*



Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

$\Rightarrow$ *linear in circuit size!*

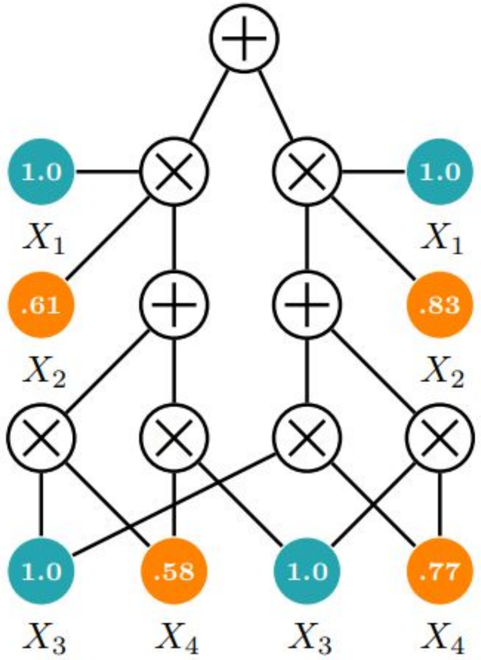
E.g. to compute $p(x_2, x_4)$:

- 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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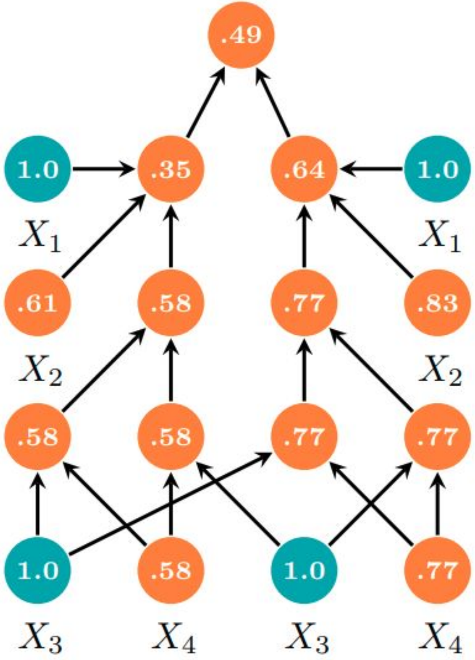
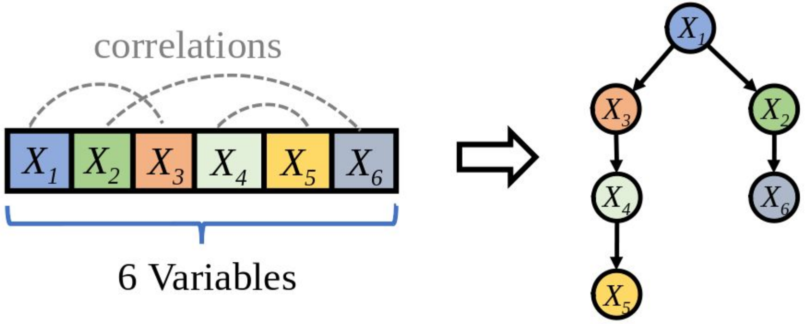


Learning Expressive Probabilistic Circuits

Hidden Chow-Liu Trees

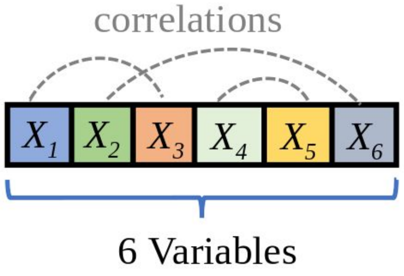
Learned **CLT structure** captures strong pairwise dependencies



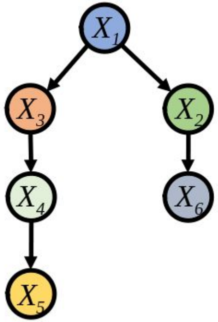
Anji Liu and Guy Van den Broeck. Tractable Regularization of Probabilistic Circuits, *NeurIPS*, 2021.

Learning Expressive Probabilistic Circuits

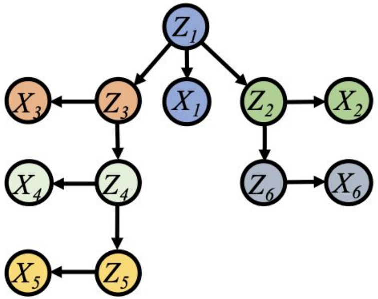
Hidden Chow-Liu Trees



Learned **CLT structure** captures strong pairwise dependencies



Learned **HCLT structure**

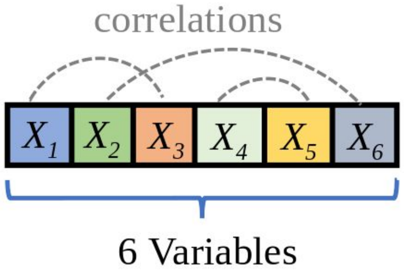


Compile into an equivalent PC

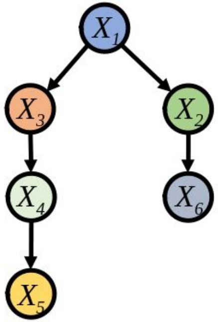
Anji Liu and Guy Van den Broeck. Tractable Regularization of Probabilistic Circuits, *NeurIPS*, 2021.

Learning Expressive Probabilistic Circuits

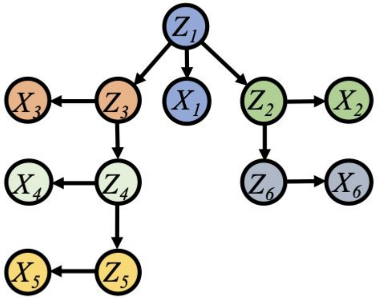
Hidden Chow-Liu Trees



Learned **CLT structure** captures strong pairwise dependencies



Learned **HCLT structure**

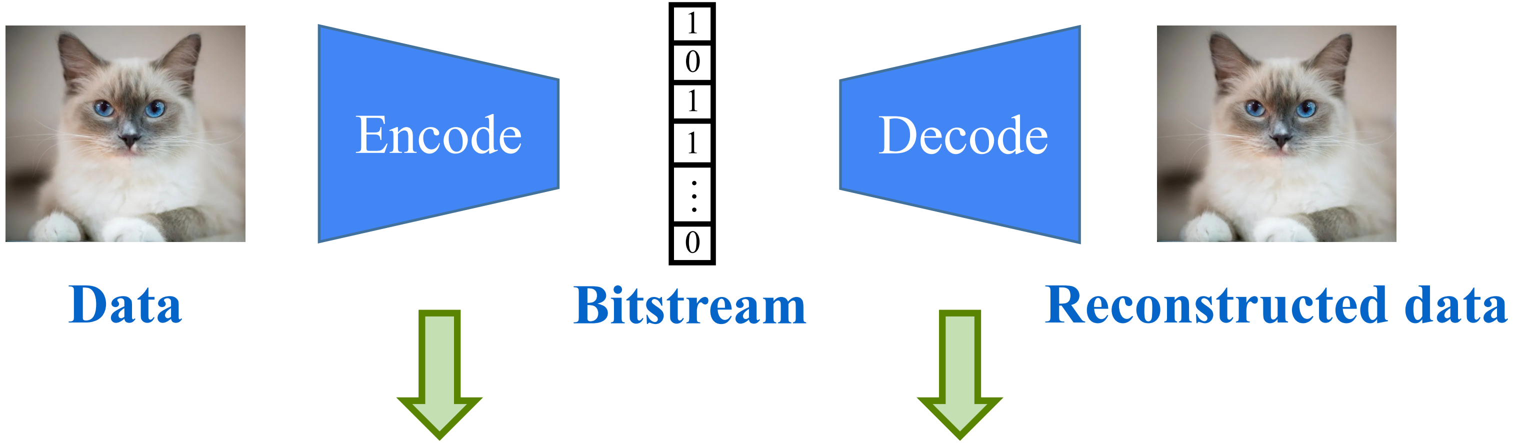


⇨ **Compile** into an equivalent PC

⇨ Mini-batch Stochastic **Expectation Maximization**

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

Lossless Data Compression



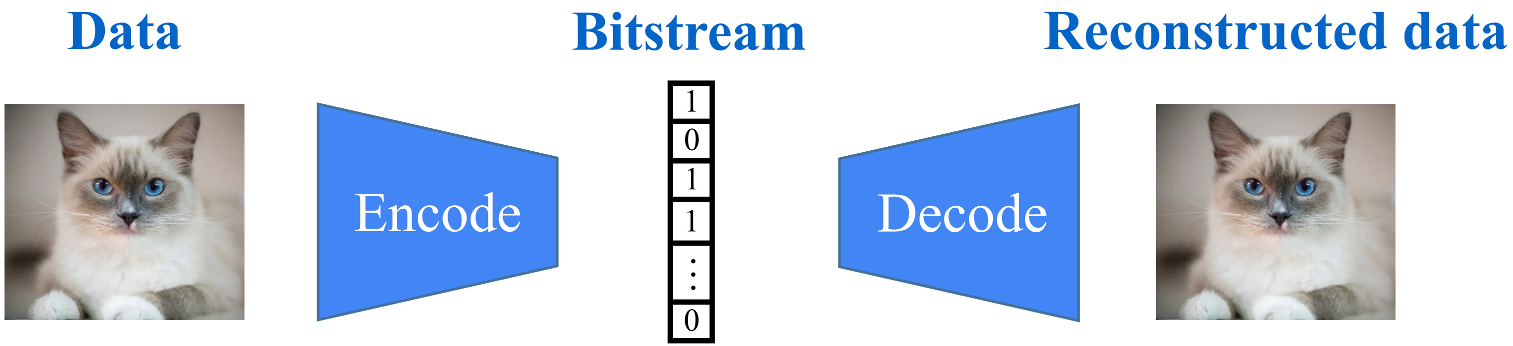
Expressive probabilistic model $p(\boldsymbol{x})$ ⇨ Determines the theoretical limit of compression rate

+

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.

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.

PC Learners keep getting better! ***… stay tuned …***

Table 1: Density estimation performance on MNIST-family datasets in test set bpd.

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

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

Meihua Dang, Anji Liu, Guy Van den Broeck, Sparse Probabilistic Circuits via Pruning and Growing, Sparsity in Neural Networks, 2022

Fully factorized

NaiveBayes AndOrGraphs PDGs

Trees PSDDs CNets LTMs SPNs NADEs

Thin Junction Trees ACs MADEs MAFs VAEs

DPPs FVSBNs TACs IAFs NAFs RAEs

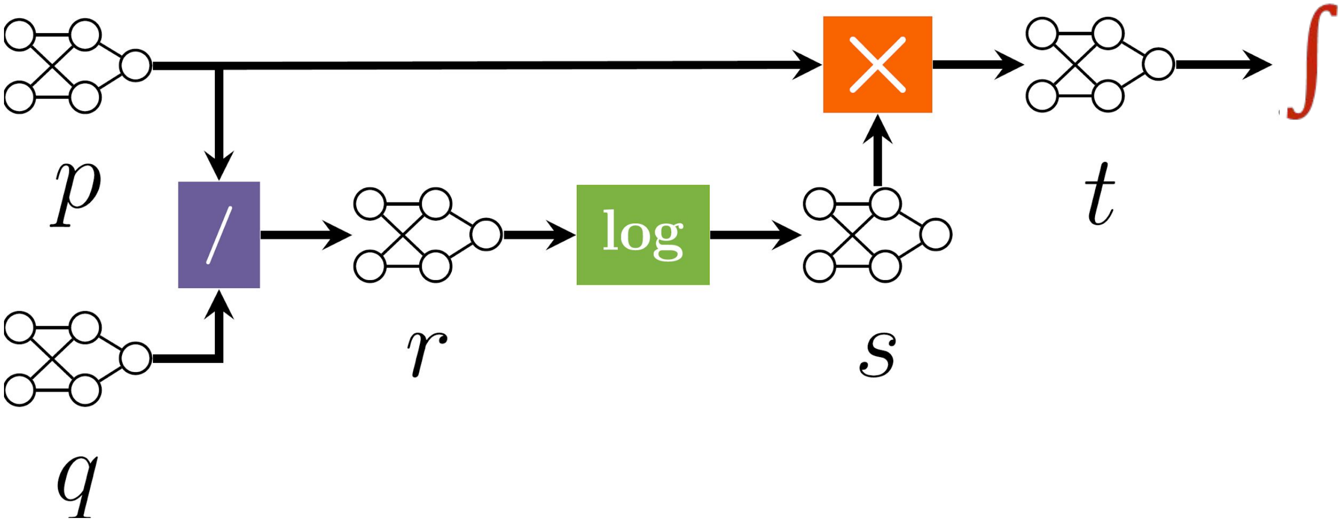
Mixtures BNs NICE FGs GANs

RealNVP MNs

Expressive models without *compromises*

Queries as pipelines: KLD

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



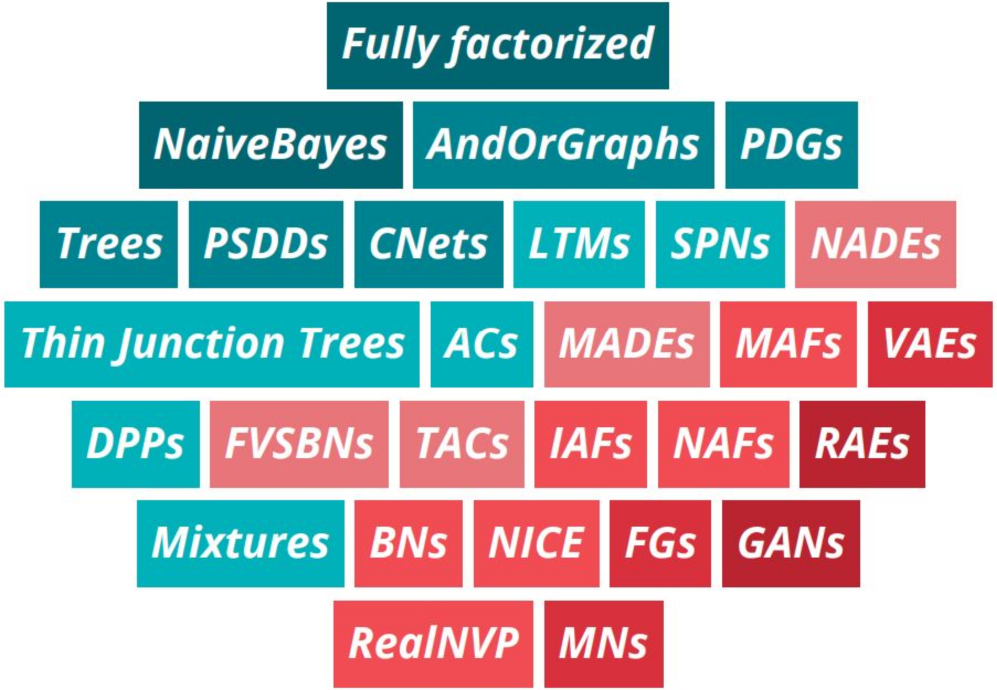
Antonio Vergari, YooJung Choi, Anji Liu, Stefano Teso and Guy Van den Broeck. A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference, *NeurIPS*, 2021.

Inference by tractable operations

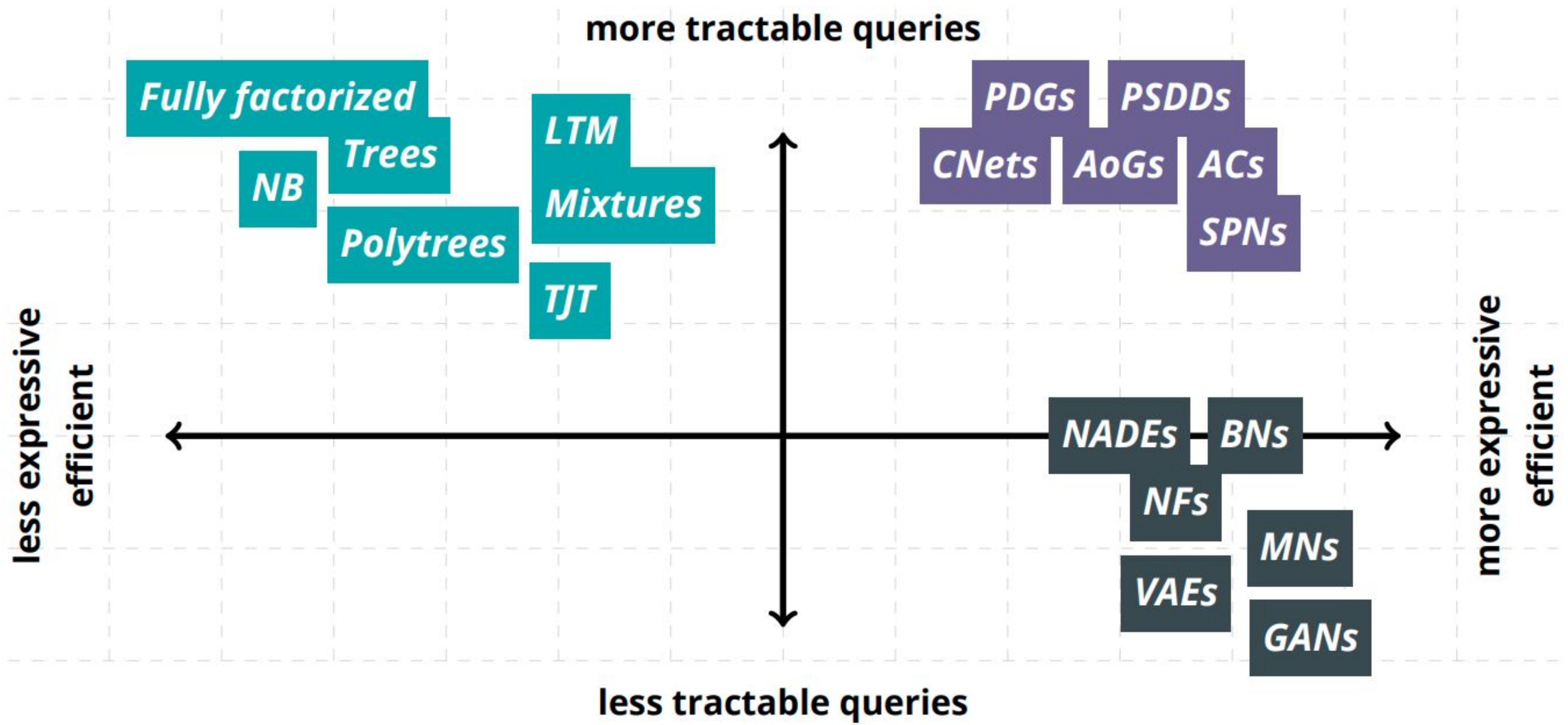
systematically derive tractable inference algorithm of complex queries

	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.



tractability is a spectrum


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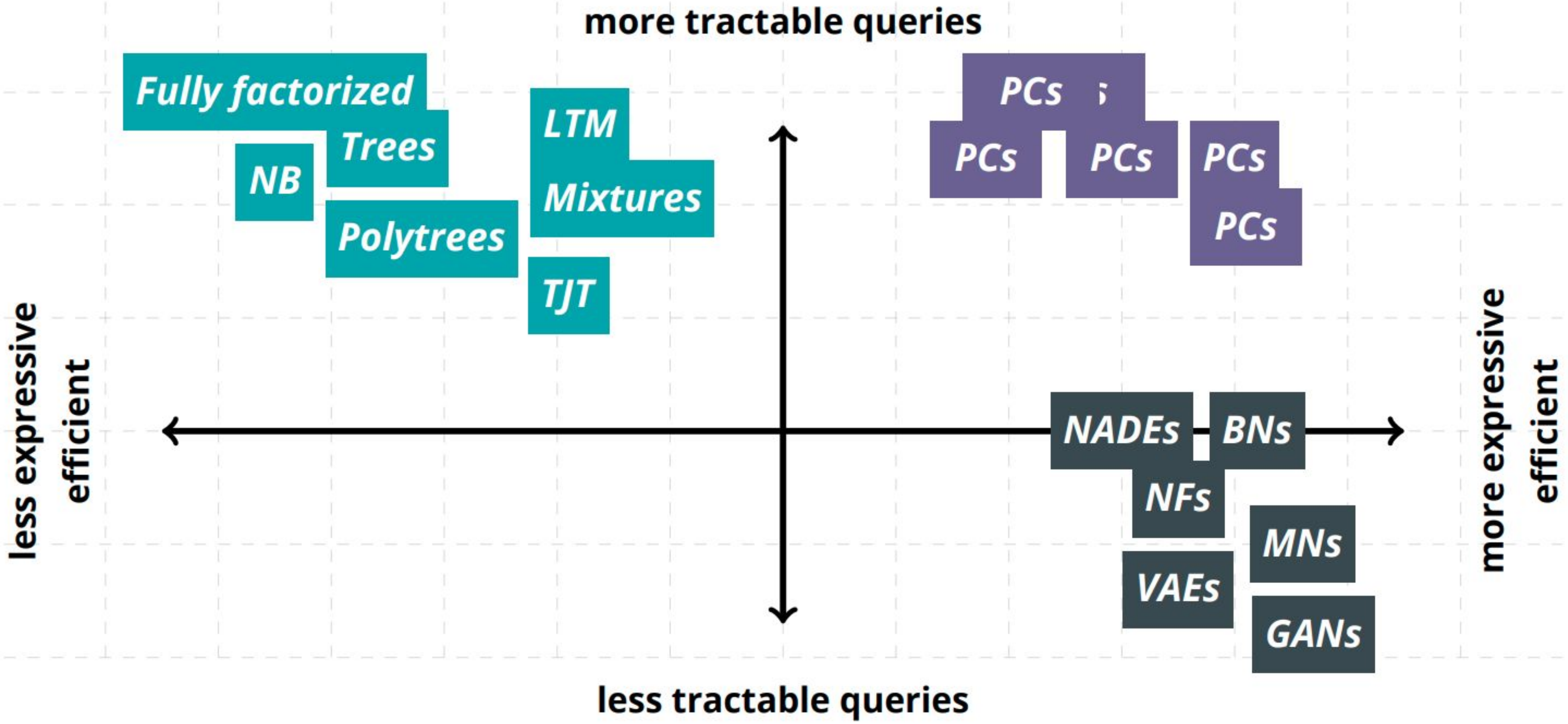
NFs
MNs
VAEs
GANs
less tractable queries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less expressive
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NFs
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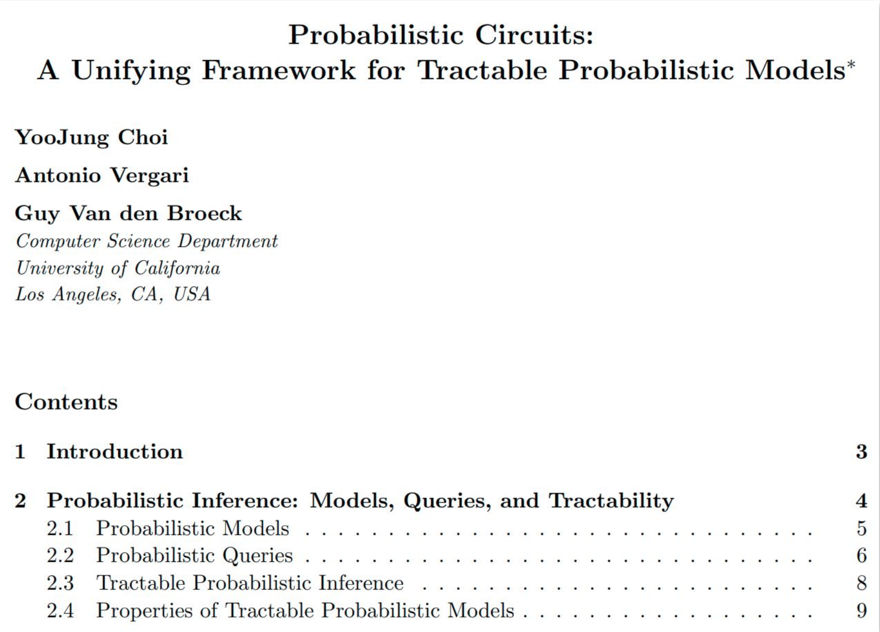
GANs
less tractable queries

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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Antonio Vergari
Guy Van den Broeck
Computer Science Department
University of California
Los Angeles, CA, USA

Contents

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

Thanks

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

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