Tractable Probabilistic Models

Representations
Inference
Learning
Applications

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based on joint AAAI-2020 and UAI-2019 tutorials with

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AoGs | PDGs | NBs | Fully factorized | sd-DNNF | PSDDs

Trees | LTMs | DNNFs | OBDDs | CNets | SPNs | NADEs

Thin Junction Trees | NNF | FBDDs | BDDs | ACs | VAEs

Polytrees | d-NNFs | ADDs | SDDs | TACs | GANs | NFs

Mixtures | XADDs | XSDDs | MNs | BNs | FGs

The Alphabet Soup of models in AI

AoGs PDGs NBs Fully factorized sd-DNNF PSDDs

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Thin Junction Trees NNF FBDDs BDDs ACs VAEs

Polytrees d-NNFs ADDs SDDs TACs GANs NFs

Mixtures XADDs XSDDs MNs BNs FGs

Logical and *Probabilistic* models

AoGs *PDGs* *NBs* *Fully factorized* *sd-DNNF* *PSDDs*

Trees *LTMs* *DNNFs* *OBDDs* *CNets* *SPNs* *NADEs*

Thin Junction Trees *NNF* *FBDDs* *BDDs* *ACs* *VAEs*

Polytrees *d-NNFs* *ADDs* *SDDs* *TACs* *GANs* *NFs*

Mixtures *XADDs* *XSDDs* *MNs* *BNs* *FGs*

Tractable and *Intractable* probabilistic models

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Mixtures XADDs XSDDs MNs BNs FGs

Expressive **models without** *compromises*

Why tractable inference?

or expressiveness vs tractability

Probabilistic circuits

a unified framework for tractable models

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or expressiveness vs tractability

Probabilistic circuits

a unified framework for tractable models

Building circuits

learning them from data and compiling other models

Applications

what are circuits useful for

Why tractable inference?

or the inherent trade-off of tractability vs. expressiveness

Why probabilistic inference?

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

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

pinterest.com/pin/190417890473268205/

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$\Longrightarrow$ ~~fitting a predictive model!~~

$\Longrightarrow$ answering probabilistic ***queries*** on a probabilistic model of the world $\mathbf{m}$

$$\mathbf{q}_1(\mathbf{m}) = \textbf{?} \qquad \mathbf{q}_2(\mathbf{m}) = \textbf{?}$$

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$\Longrightarrow$ ***marginals***

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$\mathbf{q}_2$: *Which day is most likely to have a traffic jam on my route to work?*

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$$\mathbf{q}_2(\mathbf{m}) = \mathrm{argmax}_{\mathsf{d}}\, p_{\mathbf{m}}(\mathsf{Day} = \mathsf{d} \wedge \bigvee_{i \in \mathsf{route}} \mathsf{Jam}_{\mathsf{Str}i})$$

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$\Longrightarrow$ ***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* $\mathbf{q} \in \mathcal{Q}$ *and model* $\mathbf{m} \in \mathcal{M}$ ***exactly*** *computing* $\mathbf{q}(\mathbf{m})$ *runs in time* $O(\mathrm{poly}(|\mathbf{q}| \cdot |\mathbf{m}|))$.

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$\Longrightarrow$ *think of* $|\mathbf{m}|$ *as the number of streets on my route to work*

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

What about approximate inference?

- Why approximate when we can do exact?

  $\Longrightarrow$ *and do we lose some expressiveness?*

- Approximations can be intractable as well *[Dagum et al. 1993; Roth 1996]*

  $\Longrightarrow$ *But sometimes approximate inference comes with guarantees*

- Approximate inference by exact inference in approximate model

  [Dechter et al. 2002; Choi et al. 2010; Lowd et al. 2010; Sontag et al. 2011; Friedman et al. 2018]

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Stay Tuned For ...

Next:

1. *What are classes of queries?*
2. *Are my favorite models tractable?*
3. *Are tractable models expressive?*

After: *We introduce* **probabilistic circuits** *as a unified framework for tractable probabilistic modeling*

Complete evidence queries (EVI)

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

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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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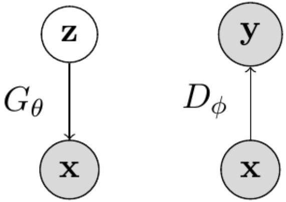
Generative Adversarial Networks

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



Goodfellow et al., "Generative adversarial nets", 2014

~~Generative Adversarial Networks~~

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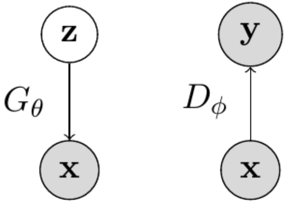
- no explicit likelihood!
  - $\Longrightarrow$ *adversarial training instead of MLE*
    - $\Longrightarrow$ *no tractable EVI*
- good sample quality
  - $\Longrightarrow$ *but lots of samples needed for MC*
- unstable training $\Longrightarrow$ *mode collapse*



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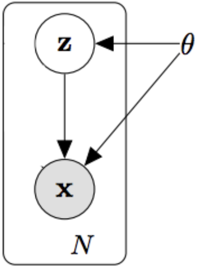
Variational Autoencoders

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

- an explicit likelihood model!



Rezende et al., *"Stochastic backprop. and approximate inference in deep generative models"*, 2014

Kingma et al., *"Auto-Encoding Variational Bayes"*, 2014

~~Variational Autoencoders~~

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

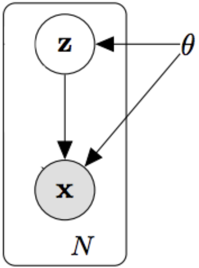
- an explicit likelihood model!
- ... but computing $\log p_\theta(\mathbf{x})$ is intractable

  $\Longrightarrow$ *an infinite and uncountable mixture*

  $\Longrightarrow$ *no tractable EVI*
- we need to optimize the ELBO...

  $\Longrightarrow$ *which is "broken"*

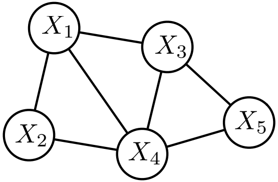
  [Alemi et al. 2017; Dai et al. 2019]



Probabilistic Graphical Models (PGMs)

Declarative semantics: a clean separation of modeling assumptions from inference

Nodes: random variables
Edges: dependencies



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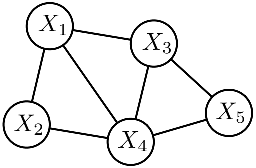
Inference:

- 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]*

PGMs: MNs and BNs

Markov Networks (MNs)

$p(\mathbf{X}) = \frac{1}{Z} \prod_c \phi_c(\mathbf{X}_c)$



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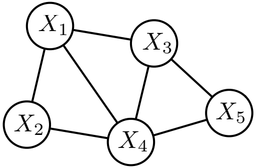
$\Longrightarrow$ EVI *queries are intractable!*



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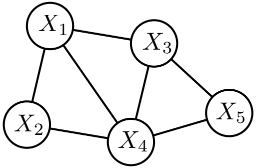
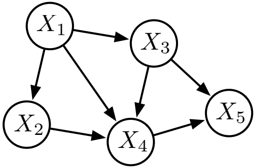


Bayesian Networks (BNs)

$$p(\mathbf{X}) = \prod_i p(X_i \mid \mathsf{pa}(X_i))$$

$\Longrightarrow$ EVI *queries are tractable!*



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 Herzl Str.?*

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

where $\mathbf{E} \subset \mathbf{X}$

$$\mathbf{H} = \mathbf{X} \setminus \mathbf{E}$$

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Conditional queries (CON)

q_4: *What is the probability that there is a traffic jam on Herzl Str.* ***given that*** *today is a Monday?*

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If you can answer MAR queries,
then you can also do ***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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Complexity of MAR on PGMs

Exact complexity: Computing MAR and COND is *#P-complete* [Cooper 1990; Roth 1996].

Approximation complexity: Computing MAR and COND approximately within a relative error of $2^{n^{1-\epsilon}}$ for any fixed ϵ is *NP-hard* [Dagum et al. 1993; Roth 1996].

Treewidth: Informally, how tree-like is the graphical model $\mathbf{m}$?
Formally, the minimum width of any tree-decomposition of $\mathbf{m}$.

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

$\Longrightarrow$ *what about bounding the treewidth by design?*

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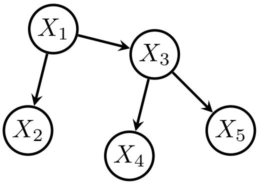
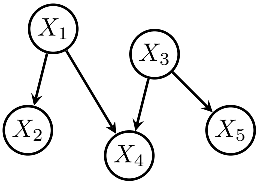
Low-treewidth PGMs



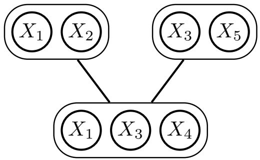
Trees

[Meilă et al. 2000]



Polytrees

[Dasgupta 1999]



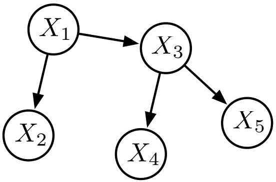
Thin Junction trees

[Bach et al. 2001]

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

Low-treewidth PGMs: trees

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



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

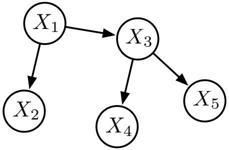
Exact querying: EVI, MAR, CON tasks *linear* for trees: $O(|\mathbf{X}|)$

Exact learning from d examples takes $O(|\mathbf{X}|^2 \cdot d)$ with the classical Chow-Liu algorithm[1]

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

What do we lose?

Expressiveness: Ability to compactly represent rich and complex classes of distributions

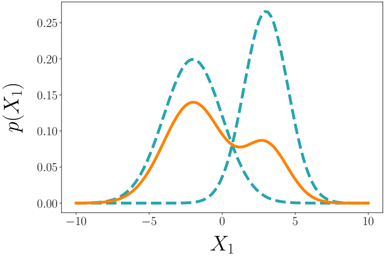


Bounded-treewidth PGMs lose the ability to represent *all possible distributions* ...

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

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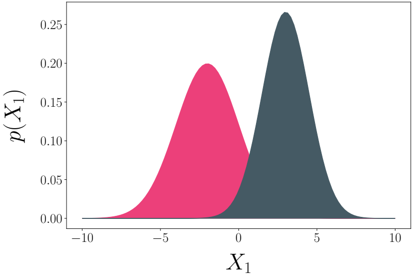

$$
\begin{aligned}
p(X) =\,& p(Z = \boxed{1}) \cdot p_1(X|Z = \boxed{1}) \\
&+ p(Z = \boxed{2}) \cdot p_2(X|Z = \boxed{2})
\end{aligned}
$$

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

$\Rightarrow$ *increased expressiveness*

Expressiveness and efficiency

Expressiveness: Ability to compactly represent rich and effective classes of functions

$\Longrightarrow$ *mixture of Gaussians can approximate any distribution!*

Expressive efficiency (succinctness) compares model sizes in terms of their ability to compactly represent functions

$\Longrightarrow$ *but how many components do they need?*

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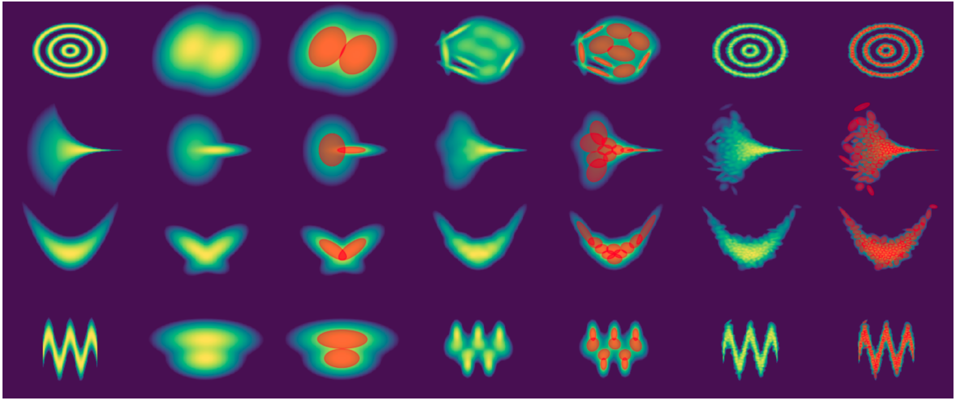
Mixture models

Expressive efficiency



⇒ *deeper mixtures would be efficient compared to shallow ones*

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?*

pinterest.com/pin/190417890473268205/

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$$\mathbf{q}_5(\mathbf{m}) = \operatorname{argmax}_{\mathbf{j}}\, p_{\mathbf{m}}(\mathbf{j}_1, \mathbf{j}_2, \ldots \mid \mathsf{Day}=\mathsf{M}, \mathsf{Time}=9)$$

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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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Maximum A Posteriori (MAP)

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$\mathbf{q}_5$: *Which combination of roads is most likely to be jammed on Monday at 9am?*

...intractable for latent variable models!

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

pinterest.com/pin/190417890473268205/

Marginal MAP (MMAP)

aka Bayesian Network MAP

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$\Rightarrow$ *NP^{PP}-complete [Park et al. 2006]*

$\Rightarrow$ *NP-hard for trees [Campos 2011]*

$\Rightarrow$ *NP-hard even for Naive Bayes [ibid.]*

pinterest.com/pin/190417890473268205/

Advanced queries

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

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Bekker et al., "Tractable Learning for Complex Probability Queries", 2015

Advanced queries

$\mathbf{q}_2$: *Which day is most likely to have a traffic jam on my route to work?*

$$\mathbf{q}_2(\mathbf{m}) = \mathrm{argmax}_{\mathsf{d}}\, p_{\mathbf{m}}(\mathsf{Day} = \mathsf{d} \wedge \bigvee_{i \in \mathsf{route}} \mathsf{Jam}_{\mathsf{Str}\ i})$$

$\Longrightarrow$ **marginals + MAP + logical events**

pinterest.com/pin/190417890473268205/

Bekker et al., "Tractable Learning for Complex Probability Queries", 2015

Advanced queries

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

q_7: *What is the probability of seeing more traffic jams in Jaffa than Marina?*

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Advanced queries

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

q_7: *What is the probability of seeing more traffic jams in Jaffa than Marina?*

$\Rightarrow$ **counts + group comparison**

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Advanced queries

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

q_7: *What is the probability of seeing more traffic jams in Jaffa than Marina?*

and more:

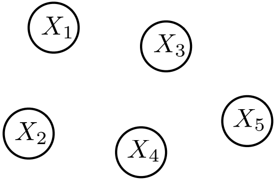
- expected classification agreement *[Oztok et al. 2016; Choi et al. 2017, 2018]*
- expected predictions *[Khosravi et al. 2019a]*

pinterest.com/pin/190417890473268205/

Bekker et al., "Tractable Learning for Complex Probability Queries", 2015

Fully factorized models

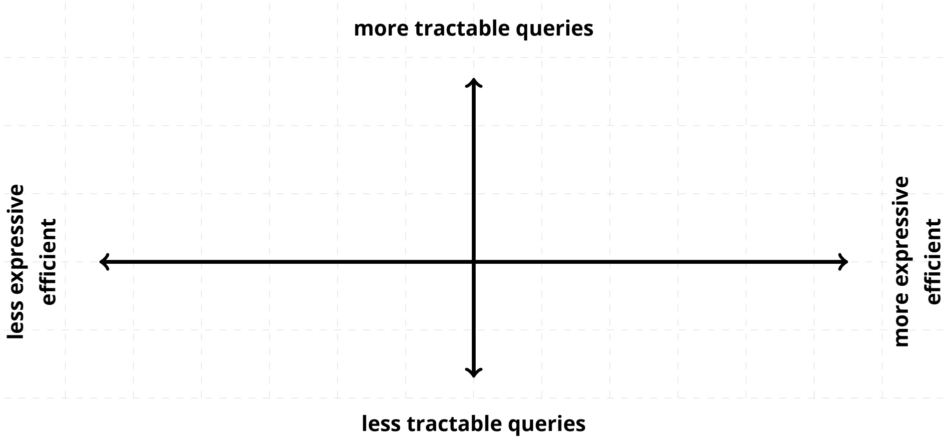
A completely disconnected graph. Example: Product of Bernoullis (PoBs)

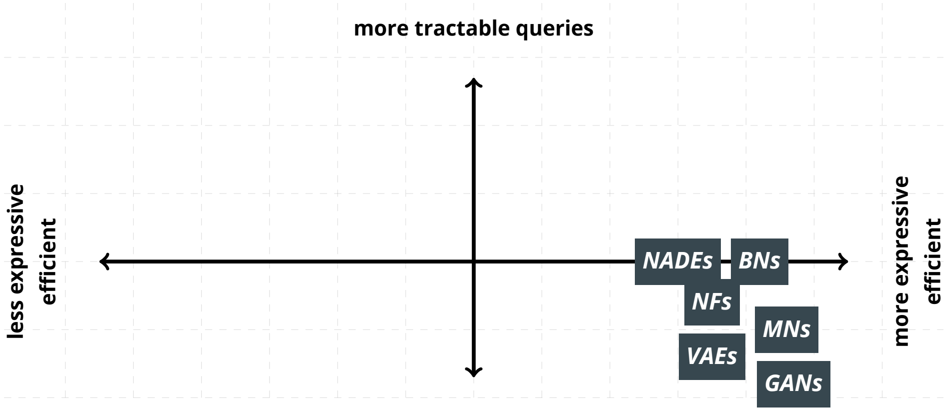


$$p(\mathbf{X}) = \prod_{i=1}^{n} p(x_i)$$

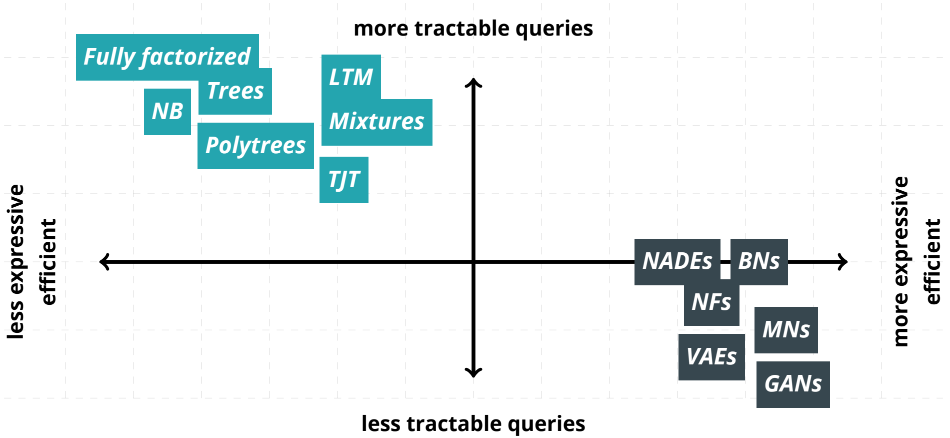
Complete evidence, marginals and MAP, MMAP inference is ***linear***!

$\Rightarrow$ *but definitely not expressive...*

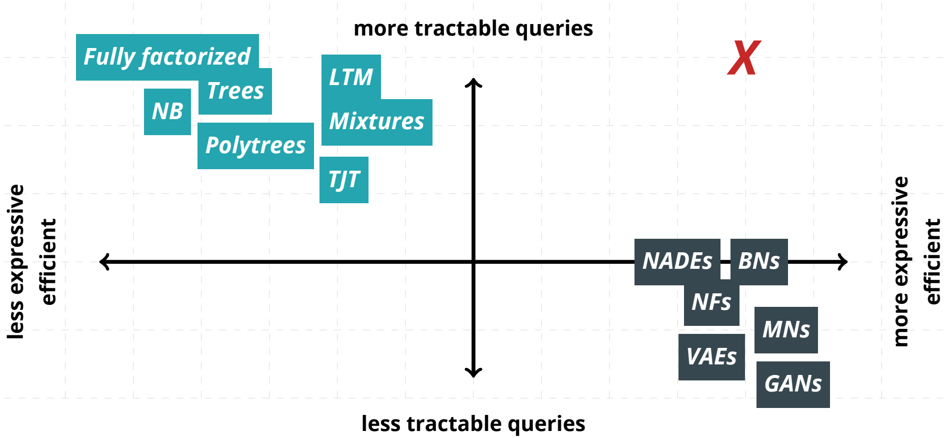

more tractable queries
less expressive
efficient
more expressive
efficient
less tractable queries



Expressive models are not very tractable...



and tractable ones are not very expressive...



probabilistic circuits are at the "sweet spot"

Probabilistic Circuits

Stay Tuned For ...

Next:

1. *What are the building blocks of tractable models?*

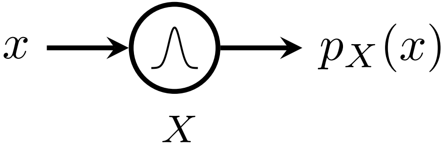
   $\Rightarrow$ *a computational graph forming a probabilistic circuit*

2. For which queries are probabilistic circuits tractable?

   $\Rightarrow$ *tractable classes induced by structural properties*

After: *How are probabilistic circuits related to the alphabet soup of models?*

Base Case: Univariate Distributions



Generally, univariate distributions are tractable for:

- EVI: output $p(X_i)$ (density or mass)
- MAR: output 1 (normalized) or Z (unnormalized)
- MAP: output the mode

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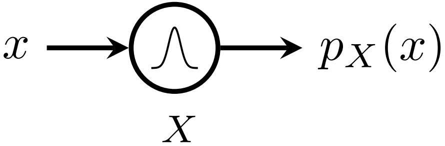

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$\Longrightarrow$ *for example, X or $\neg X$ for Boolean random variable*

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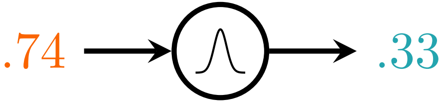

X

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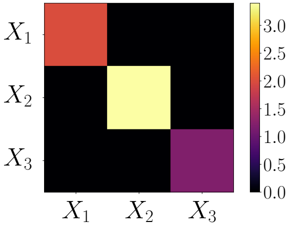
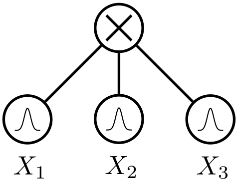
Factorizations are products

Divide and conquer complexity

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





$\Longrightarrow$ *e.g. modeling a multivariate Gaussian with diagonal covariance matrix*

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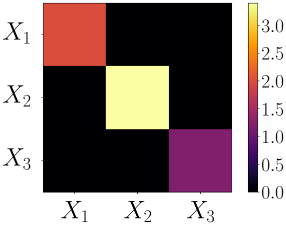

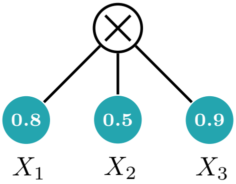

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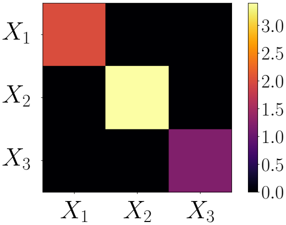

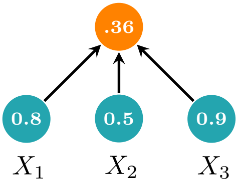

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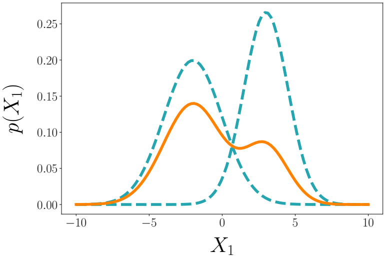
Mixtures are sums

Also mixture models can be treated as a simple ***computational unit*** over distributions



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

Mixtures are sums

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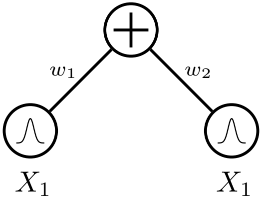

$$p(x) = 0.2 \cdot p_1(x) + 0.8 \cdot p_2(x)$$

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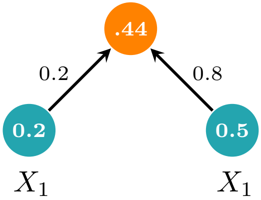


$$p(x) = 0.2 \cdot p_1(x) + 0.8 \cdot p_2(x)$$

With mixtures, we increase expressiveness

$\Longrightarrow$ *by **stacking** them we increase expressive efficiency*

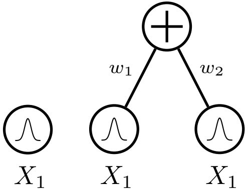
A grammar for tractable models

Recursive semantics of probabilistic circuits

X_1

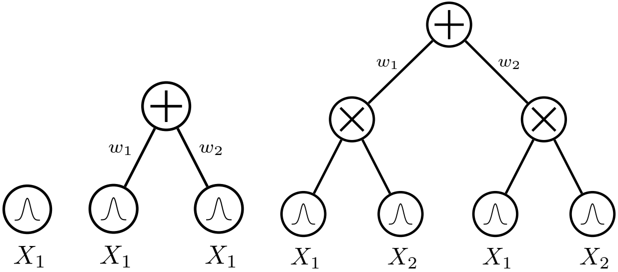
A grammar for tractable models

Recursive semantics of probabilistic circuits



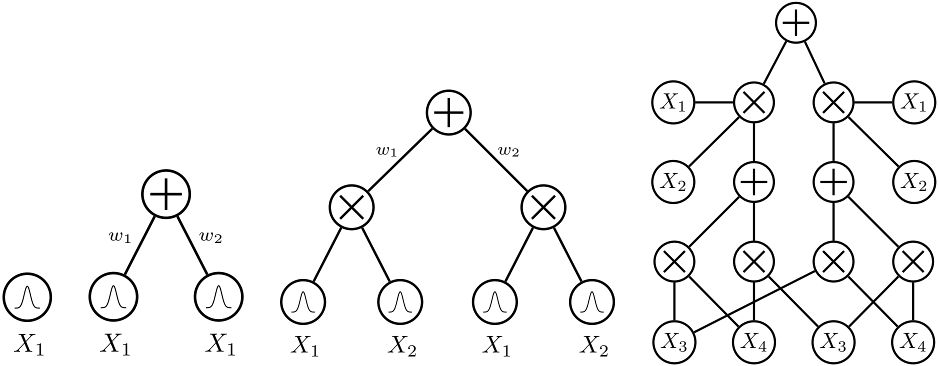
A grammar for tractable models

Recursive semantics of probabilistic circuits



A grammar for tractable models

Recursive semantics of probabilistic circuits



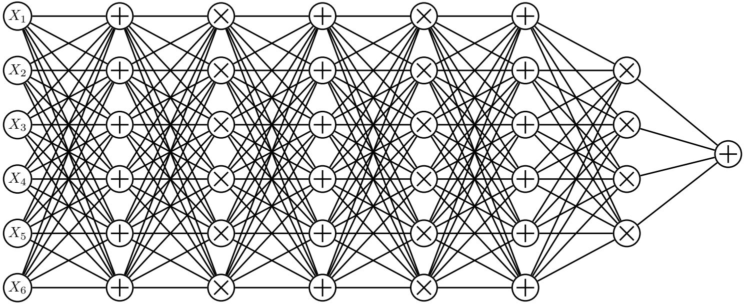
Probabilistic circuits are not PGMs!

They are ***probabilistic*** and ***graphical***, however …

	PGMs	***Circuits***
Nodes:	random variables	unit of computations
Edges:	dependencies	order of execution
Inference:	conditioning elimination message passing	feedforward pass backward pass

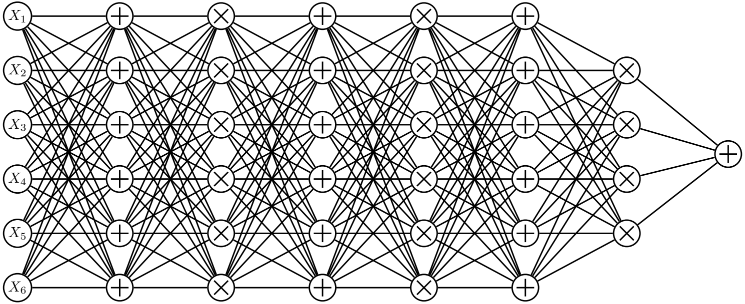
$\Longrightarrow$ *they are computational graphs, more like neural networks*

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!*~~

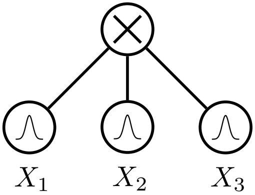
$\Longrightarrow$ structural constraints needed for tractability

How do we ensure tractability?

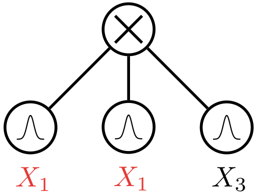
Decomposability

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

$\Rightarrow$ *just like in factorization!*



decomposable circuit



non-decomposable circuit

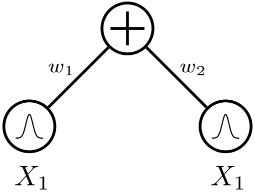
Darwiche et al., "A knowledge compilation map", 2002

Smoothness

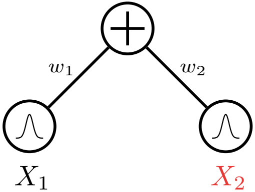
aka completeness

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

$\Longrightarrow$ *otherwise not accounting for some variables*



smooth circuit



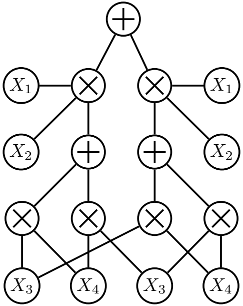
non-smooth circuit

$\Longrightarrow$ *smoothness can be easily enforced [Shih et al. 2019]*

Darwiche et al., "A knowledge compilation map", 2002

Tractable MAR/CON

Smoothness and decomposability enable tractable MAR/CON queries



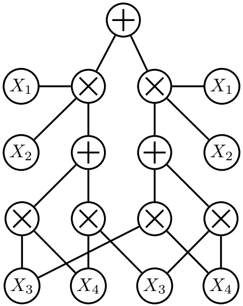
Tractable MAR/CON

Smoothness and decomposability enable tractable MAR/CON queries

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

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

$\Longrightarrow$ *larger integrals decompose into easier ones*



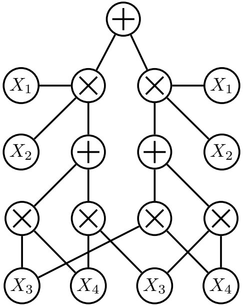
Tractable MAR/CON

Smoothness and decomposability enable tractable MAR/CON queries

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*

Tractable MAR/CON

Smoothness and decomposability enable tractable MAR/CON queries

Forward pass evaluation for MAR

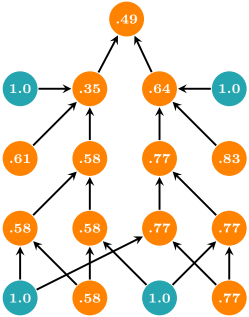
$\Longrightarrow$ *linear in circuit size!*

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

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

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

- leafs over X_2 and X_4 output EVI

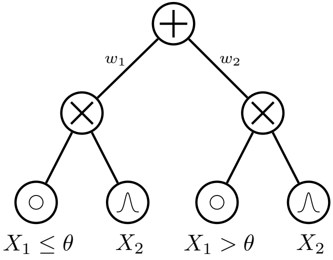


Determinism

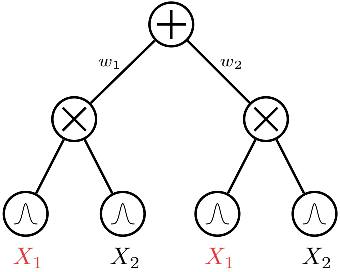
aka selectivity

A sum node is deterministic if the output of only one children is non zero for any input

$\Longrightarrow$ *e.g. if their distributions have disjoint support*



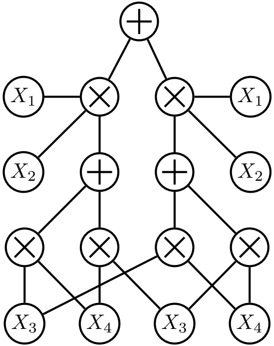
deterministic circuit



non-deterministic circuit

Tractable MAP

The addition of determinism enables tractable MAP queries!



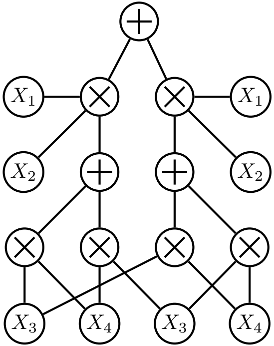
Tractable MAP

The addition of determinism enables tractable MAP queries!

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):

$$\begin{aligned}
\operatorname*{argmax}_{\mathbf{q}} p(\mathbf{q} \mid \mathbf{e}) &= \operatorname*{argmax}_{\mathbf{q}} p(\mathbf{q}, \mathbf{e}) \\
&= \operatorname*{argmax}_{\mathbf{q_x}, \mathbf{q_y}} p(\mathbf{q_x}, \mathbf{e_x}, \mathbf{q_y}, \mathbf{e_y}) \\
&= \operatorname*{argmax}_{\mathbf{q_x}} p(\mathbf{q_x}, \mathbf{e_x}), \operatorname*{argmax}_{\mathbf{q_y}} p(\mathbf{q_y}, \mathbf{e_y})
\end{aligned}$$

$\Longrightarrow$ *solving optimization independently*



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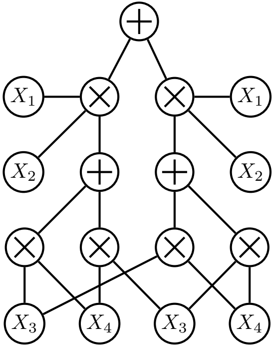
If $p(\mathbf{q},\mathbf{e}) = \sum_i w_i p_i(\mathbf{q},\mathbf{e}) = \max_i w_i p_i(\mathbf{q},\mathbf{e})$,
(***deterministic*** sum node):

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

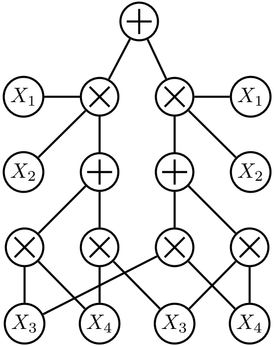
$\Rightarrow$ *one non-zero child term, thus sum is max*



Tractable MAP

The addition of determinism enables tractable MAP queries!

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



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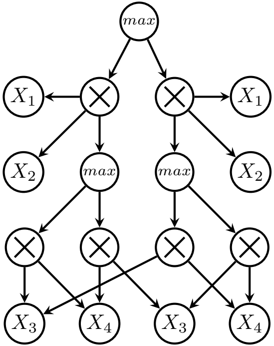
In practice:

1. turn sum into max nodes
2. evaluate $p(\mathbf{e})$ bottom-up
3. retrieve max activations top-down
4. compute MAP queries at leaves



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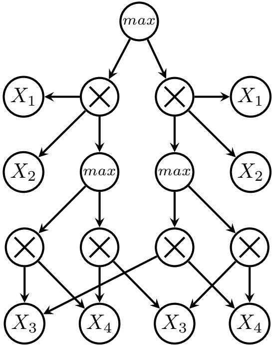


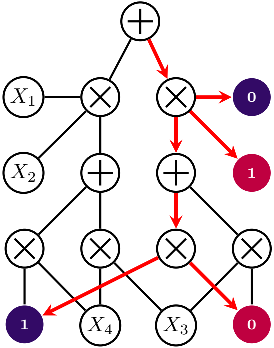
Tractable MAP

The addition of determinism enables tractable MAP queries!

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

In practice:

1. turn sum into max nodes
2. evaluate $p(\mathbf{e})$ bottom-up
3. retrieve max activations top-down
4. compute MAP queries at leaves



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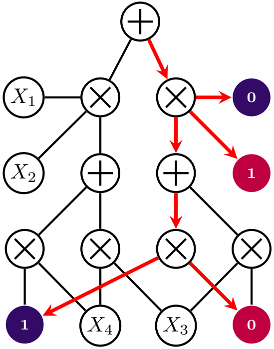


In practice:

1. turn sum into max nodes
2. evaluate $p(\mathbf{e})$ bottom-up
3. retrieve max activations top-down
4. compute MAP queries at leaves

Approximate MAP

If the probabilistic circuit is ***non-deterministic***, MAP is intractable:

$\Rightarrow$ *e.g. with latent variables* $\mathbf{Z}$

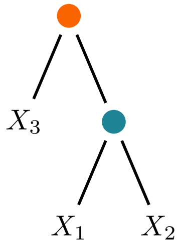
$$\operatorname*{argmax}_{\mathbf{q}} \sum_{i} w_i p_i(\mathbf{q}, \mathbf{e}) = \operatorname*{argmax}_{\mathbf{q}} \sum_{\mathbf{z}} p(\mathbf{q}, \mathbf{z}, \mathbf{e}) \neq \operatorname*{argmax}_{\mathbf{q}} \max_{\mathbf{z}} p(\mathbf{q}, \mathbf{z}, \mathbf{e})$$

However, same two steps algorithm, still used as an approximation to MAP *[Liu et al. 2013; Peharz et al. 2016]*

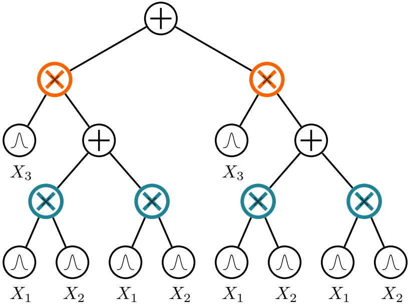
Structured decomposability

A product node is structured decomposable if decomposes according to a node in a ***vtree***

$\Rightarrow$ *stronger requirement than decomposability*



vtree



structured decomposable circuit

Structured decomposability enables tractable ...

- ***Entropy*** of probabilistic circuit *[Liang et al. 2017b]*
- ***Symmetric*** and ***group queries*** (exactly-k, odd-number, more, etc.) *[Bekker et al. 2015]*

For the "right" vtree

- Probability of logical circuit event in probabilistic circuit *[ibid.]*
- ***Multiply*** two probabilistic circuits *[Shen et al. 2016]*
- ***KL Divergence*** between probabilistic circuits *[Liang et al. 2017b]*
- ***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]*

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- ***Expected predictions*** *[Khosravi et al. 2019b]*

Stay Tuned For ...

Next:

1. *How probabilistic circuits are related to logical ones?*

   $\Longrightarrow$ *a historical perspective*

2. *How probabilistic circuits in the literature relate and differ?*

   $\Longrightarrow$ *SPNs, ACs, CNets, PSDDs*

3. *How classical tractable models can be turned in a circuit?*

   $\Longrightarrow$ *Compiling low-treewidth PGMs*

After: *How do I build my own probabilistic circuit?*

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:

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

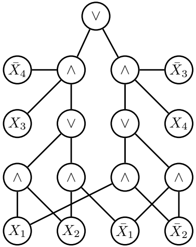
$\Longrightarrow$ *Algebraic model counting [Kimmig et al. 2017], Semi-ring programming [Belle et al. 2016]*

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

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

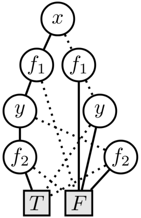
$\Longrightarrow$ *logical circuits!*

Logical circuits



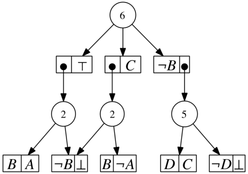
s/d-D/NNFs

[Darwiche et al. 2002]



O/BDDs

[Bryant 1986]



SDDs

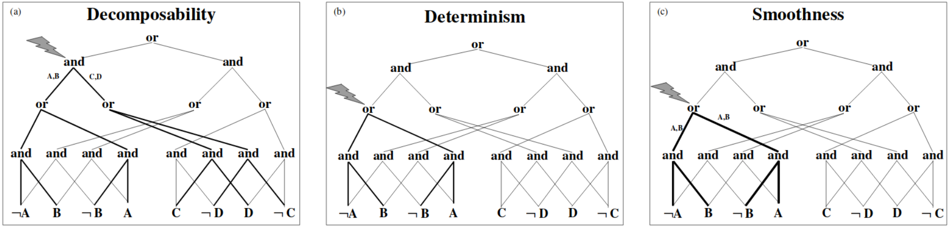
[Darwiche 2011]

Logical circuits are compact representations for boolean functions...

Logical circuits

structural properties

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

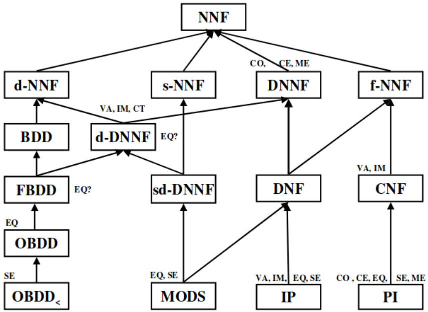


Darwiche et al., “A knowledge compilation map”, 2002

Logical circuits

a knowledge compilation map

...inducing ***a hierarchy of tractable query classes***



Darwiche et al., "A knowledge compilation map", 2002

Logical circuits

connection to probabilistic circuits through WMC

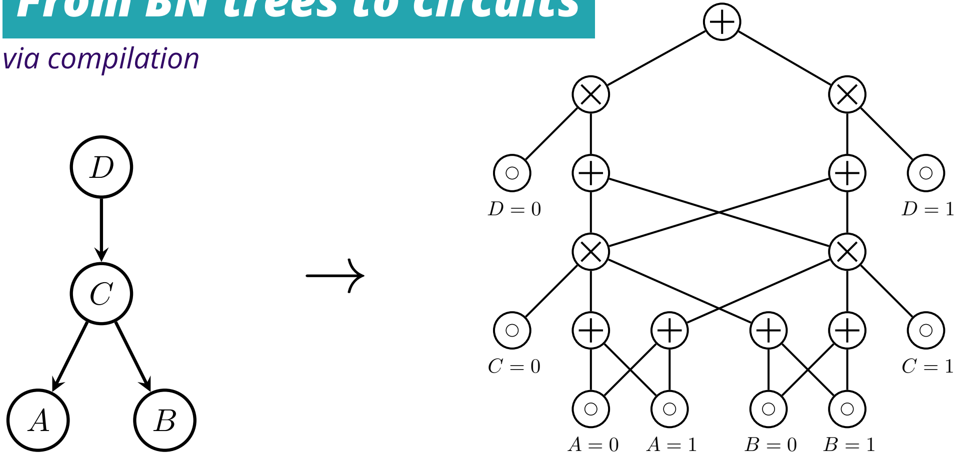
- A task called ***weighted model counting*** (**WMC**)

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

- Two decades worth of connections:
  1. Encode probabilistic model as WMC (add variable placeholders for parameters)
  2. Compile Δ into a d-DNNF (or OBDD, SDD, etc.)
  3. Tractable MAR/CON by tractable WMC on circuit
  4. Depending on the WMC encoding even tractable MAP
- End result equivalent to probabilistic circuit: efficiently replace parameter variables in logical circuit by edge parameters in probabilistic circuit

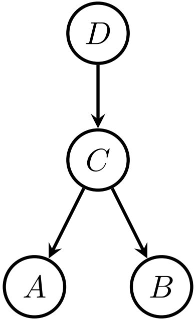
From BN trees to circuits

via compilation



From BN trees to circuits

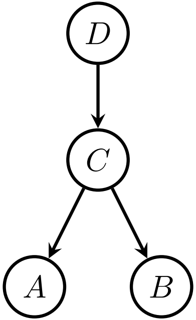
via compilation



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

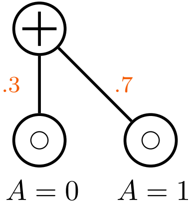
From BN trees to circuits

via compilation



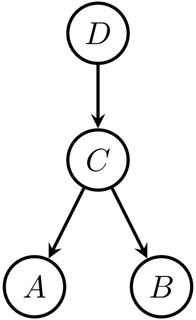
...compile a leaf CPT

$p(A|C=0)$



From BN trees to circuits

via compilation



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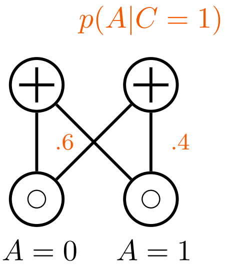
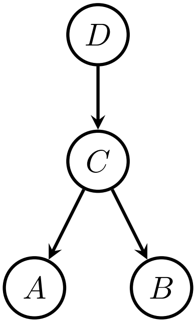
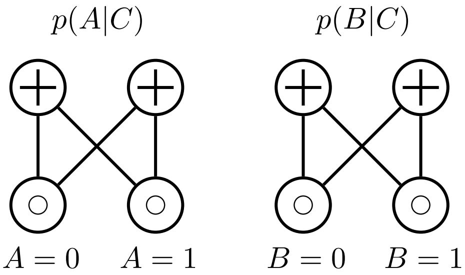


From BN trees to circuits

via compilation



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



From BN trees to circuits

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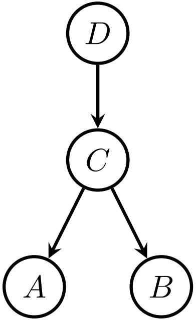
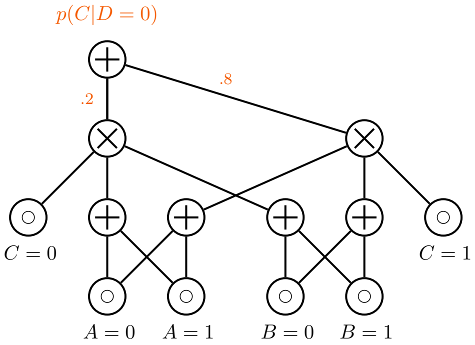


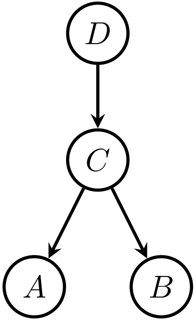
...and recurse over parents...

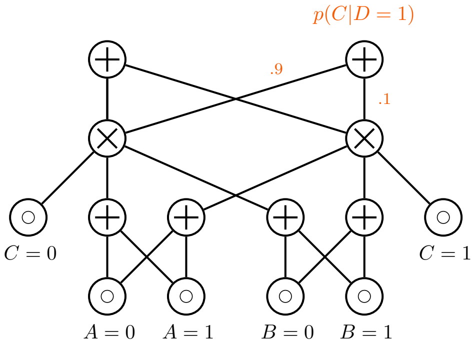


From BN trees to circuits

via compilation

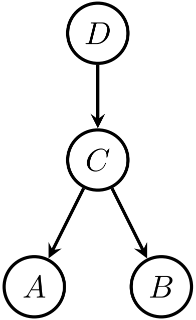
…while reusing previously compiled nodes!…

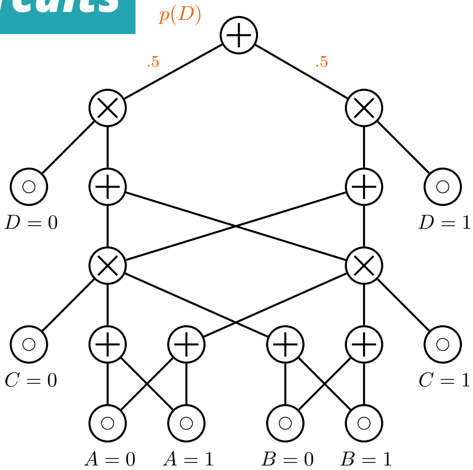




From BN trees to circuits

via compilation





Low-treewidh PGMs

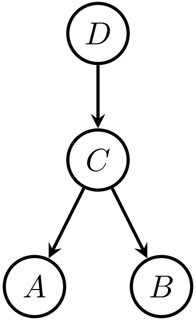
Tree, polytrees and thin junction trees can be turned into

- decomposable
- smooth
- deterministic

probabilistic circuits

Therefore they support tractable

- EVI
- MAR/CON
- MAP



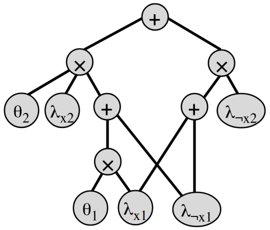
Arithmetic Circuits (ACs)

ACs *[Darwiche 2003]* are

- decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- (MAP)



$\Rightarrow$ *parameters attached to leaves (cf. WMC) ...can be moved to sum nodes*

$\Rightarrow$ *Support for tractable MAP queries depends on intended WMC encoding*

$\Rightarrow$ *Also see related AND/OR search spaces [Dechter et al. 2007]*

Lowd et al., "Learning Markov Networks With Arithmetic Circuits", 2013

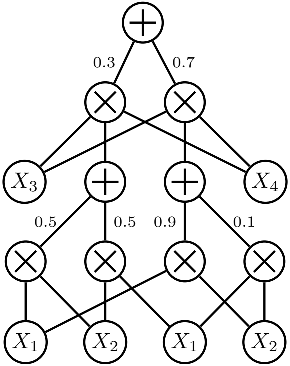
Sum-Product Networks (SPNs)

SPNs *[Poon et al. 2011]* are

- decomposable
- smooth
- ~~deterministic~~

They support tractable

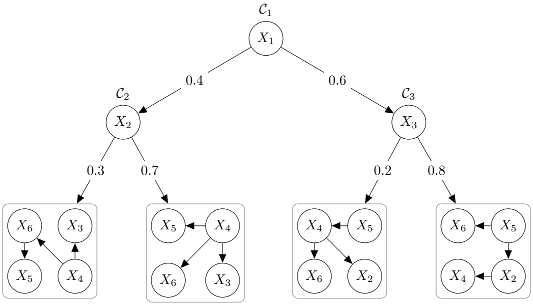
- EVI
- MAR/CON
- ~~MAP~~



$\Longrightarrow$ *deterministic SPNs are also called* selective *[Peharz et al. 2014]*

Cutset Networks (CNets)

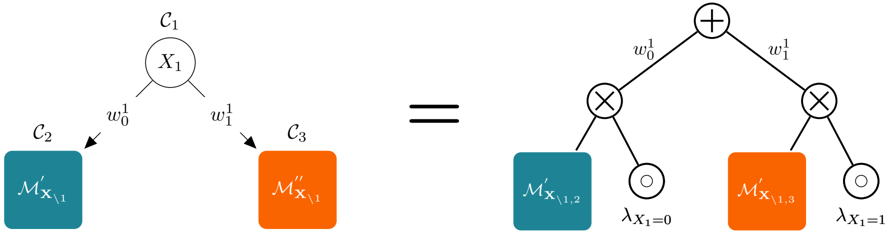
A CNet *[Rahman et al. 2014]* is a ***weighted model tree*** *[Dechter et al. 2007]* whose leaves are tree Bayesian networks



$\Longrightarrow$ *they can be represented as probabilistic circuits*

CNets as probabilistic circuits

Every ***decision node*** in the CNet can be represented as a deterministic, smooth sum node



and we can recurse on each child node until a BN tree is reached

$\Longrightarrow$ *compilable into a deterministic, smooth and decomposable circuit!*

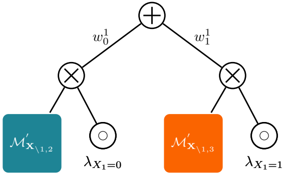
CNets as probabilistic circuits

CNets are

- decomposable
- smooth
- deterministic

They support tractable

- EVI
- MAR/CON
- MAP



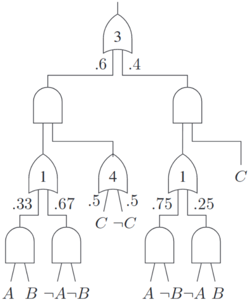
Probabilistic Sentential Decision Diagrams

PSDDs *[Kisa et al. 2014a]* are

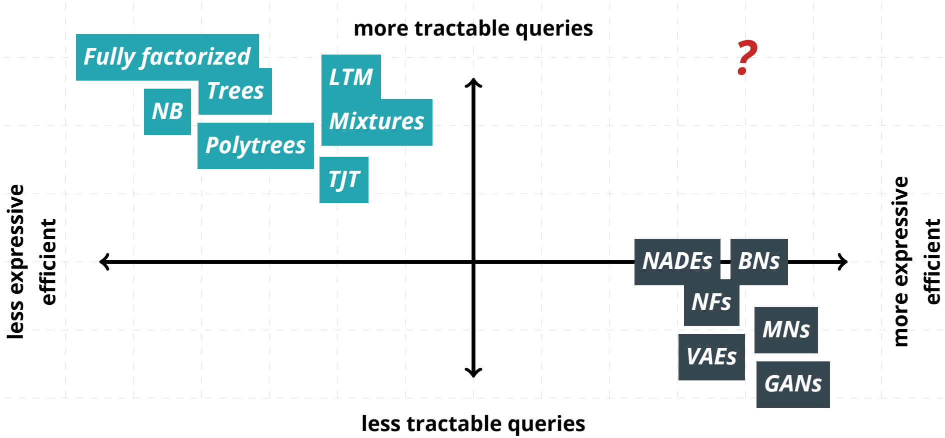
- structured decomposable
- smooth
- deterministic

They support tractable

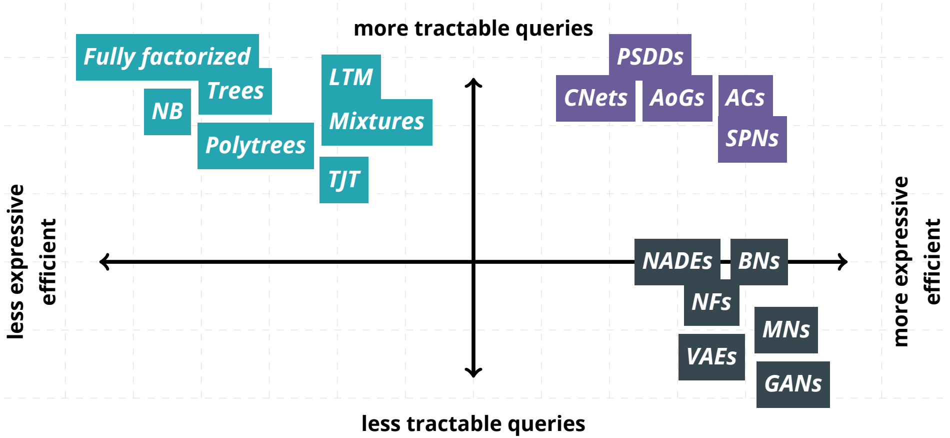
- EVI
- MAR/CON
- MAP
- Complex queries!



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



where are probabilistic circuits?



tractability vs expressive efficiency

How expressive are probabilistic circuits?

Measuring average test set log-likelihood on 20 density estimation benchmarks

Comparing against intractable models:

- Bayesian networks (BN) *[Chickering 2002]* with sophisticated context-specific CPDs
- MADEs *[Germain et al. 2015]*
- VAEs *[Kingma et al. 2014]* (IWAE ELBO *[Burda et al. 2015]*)

Gens et al., "Learning the Structure of Sum-Product Networks", 2013
Peharz et al., "Probabilistic deep learning using random sum-product networks", 2018

How expressive are probabilistic circuits?

density estimation benchmarks

dataset	best circuit	BN	MADE	VAE	dataset	best circuit	BN	MADE	VAE
nltcs	**-5.99**	-6.02	-6.04	**-5.99**	***dna***	**-79.88**	-80.65	-82.77	-94.56
msnbc	**-6.04**	**-6.04**	-6.06	-6.09	***kosarek***	**-10.52**	-10.83	-	-10.64
kdd	-2.12	-2.19	**-2.07**	-2.12	***msweb***	-9.62	-9.70	**-9.59**	-9.73
plants	**-11.84**	-12.65	-12.32	-12.34	***book***	-33.82	-36.41	-33.95	**-33.19**
audio	-39.39	-40.50	-38.95	**-38.67**	***movie***	-50.34	-54.37	-48.7	**-47.43**
jester	-51.29	**-51.07**	-52.23	-51.54	***webkb***	-149.20	-157.43	-149.59	**-146.9**
netflix	-55.71	-57.02	-55.16	**-54.73**	***cr52***	-81.87	-87.56	-82.80	**-81.33**
accidents	-26.89	**-26.32**	-26.42	-29.11	***c20ng***	-151.02	-158.95	-153.18	**-146.9**
retail	**-10.72**	-10.87	-10.81	-10.83	***bbc***	**-229.21**	-257.86	-242.40	-240.94
pumbs*	-22.15	**-21.72**	-22.3	-25.16	***ad***	-14.00	-18.35	**-13.65**	-18.81

Building circuits

Read more in online slides about ...

Building Circuits:

1. *How to learn circuit parameters?*

   $\Longrightarrow$ *convex optimization, EM, SGD, Bayesian learning, ...*

2. *How to learn the structure of circuits?*

   $\Longrightarrow$ *local search, random structures, ensembles, ...*

3. *How to compile other models to circuits?*

   $\Longrightarrow$ *PGM compilation, probabilistic databases, probabilistic programming*

See: `http://starai.cs.ucla.edu/slides/TPMTutorialUAI19.pdf`

Tractable Learning

A learner L *is a* tractable learner *for a class of queries* $\mathcal{Q}$ *iff*

(1) for any dataset $\mathcal{D}$*, learner* $L(\mathcal{D})$ *runs in time* $O(\text{poly}(|\mathcal{D}|))$*, and*

(2) outputs a probabilistic model that is tractable for queries $\mathcal{Q}$.

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$\implies$ *Guarantees learned model has size* $O(\text{poly}(|\mathcal{D}|))$

$\implies$ *Guarantees learned model has size* $O(\text{poly}(|\mathbf{X}|))$

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$\implies$ *Guarantees learned model has size* $O(\text{poly}(|\mathbf{X}|))$

(2) outputs a probabilistic model that is tractable for queries $\mathcal{Q}$.

$\implies$ *Guarantees efficient querying for* $\mathcal{Q}$ *in time* $O(\text{poly}(|\mathbf{X}|))$

Stay Tuned For ...

Next:

1. *How to learn circuit parameters?*

   $\Rightarrow$ *convex optimization, EM, SGD, Bayesian learning, ...*

2. *How to learn the structure of circuits?*

   $\Rightarrow$ *local search, random structures, ensembles, ...*

After: *What is this used for?*

Learning circuit parameters

The parameters of a probabilistic circuit are

sum node parameters $\boldsymbol{w}$ + input distributions' parameters $\boldsymbol{\theta}$

$\Longrightarrow$ *e.g., parameters of Bernoulli or Gaussian leaves*

Recall that if a sum node is **non-deterministic**, it marginalizes out latent variables Z...

$\Longrightarrow$ *i.e., we are training a mixture model*

Learning circuit parameters

deterministic circuits $\Rightarrow$ closed-form, convex optimization *[Kisa et al. 2014b; Liang et al. 2019]*

non- deterministic circuits $\Rightarrow$

- SGD *[Peharz et al. 2018]*
- soft/hard EM *[Poon et al. 2011; Peharz 2015]*
- bayesian moment matching *[Jaini et al. 2016]*
- collapsed variational Bayes *[Zhao et al. 2016a]*
- CCCP *[Zhao et al. 2016b]*
- Extended Baum-Welch *[Rashwan et al. 2018]*

Deterministic circuits

Given a deterministic circuit $\mathcal{C}$ and a complete dataset $\mathbf{D}$, the likelihood of $\mathcal{C}$ given $\mathbf{D}$ is

$$L(\boldsymbol{w}; \mathbf{D}) = \prod_{\mathbf{x} \in \mathbf{D}} p_{\mathcal{C}}(\mathbf{x}; \boldsymbol{w})$$

as it decomposes as in BNs, the MLE parameters are computable as

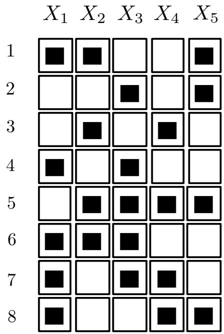
$$w_{i,j}^{\mathsf{MLE}} = \frac{\sum_{d \in \mathbf{D}} \mathbb{1}\{\mathbf{x} \models [i \wedge j]\}}{\sum_{d \in \mathbf{D}} \mathbb{1}\{\mathbf{x} \models [i]\}}$$

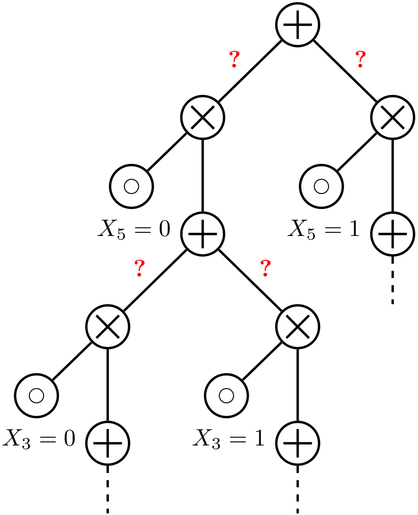
$\implies$ *compute sufficient statistics (just count) in a single pass of* $\mathbf{D}$

Kisa et al., "Probabilistic sentential decision diagrams", 2014
Liang et al., "Learning Logistic Circuits", 2019

Deterministic circuits

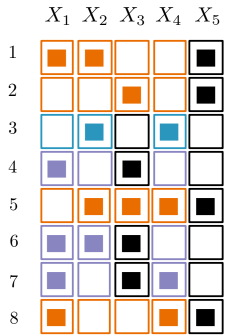
An example

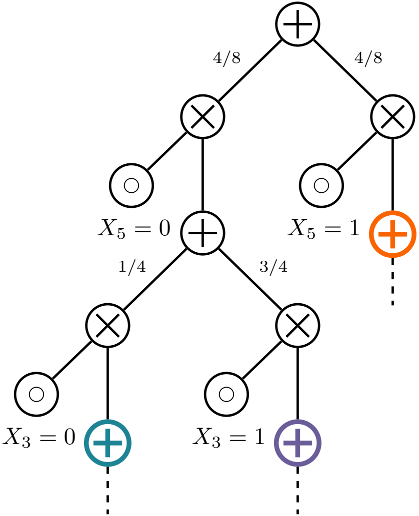




Deterministic circuits

An example





Non-deterministic circuits

Gradient Descent

Computing the likelihood gradient and optimize by GD

	Δw_{pc}
Soft Gradient	
Generative ($\nabla_{w_{pc}} S(\mathbf{x})$)	$S_c(\mathbf{x}) \nabla_{S_p(\mathbf{x})} S(\mathbf{x})$
Discriminative ($\nabla_{w_{pc}} \log S(\mathbf{y}\|\mathbf{x})$)	$\frac{\nabla_{w_{pc}} S(\mathbf{y}\|\mathbf{x})}{S(\mathbf{y}\|\mathbf{x})} - \frac{\nabla_{w_{pc}} S(*\|\mathbf{x})}{S(*\|\mathbf{x})}$
Hard Gradient	
Generative ($\nabla_{w_{pc}} \log M(\mathbf{x})$)	$\frac{\sharp\{w_{pc} \in W_{\mathbf{x}}\}}{w_{pc}}$
Discriminative ($\nabla_{w_{pc}} \log M(\mathbf{y}\|\mathbf{x})$)	$\frac{\sharp\{w_{pc} \in W_{(\mathbf{y}\|\mathbf{x})}\} - \sharp\{w_{pc} \in W_{(\mathbf{1}\|\mathbf{x})}\}}{w_{pc}}$

Gens et al., "Discriminative Learning of Sum-Product Networks", 2012

Non-deterministic circuits

Expectation Maximization

...or using EM by considering each sum node as the marginalization of a hidden variable

Soft Posterior $(p(H_p = c\|\mathbf{x}))$	$\propto$	$\frac{1}{S(\mathbf{x})} \frac{\partial S(\mathbf{x})}{\partial S_p(\mathbf{x})} S_c(\mathbf{x}) w_{pc}$
Hard Posterior $(p(H_p = c\|\mathbf{x}))$	$=$	$\begin{cases} 1 \text{ if } w_{pc} \in W_{\mathbf{x}} \\ 0 \text{ otherwise} \end{cases}$

Peharz et al., "On the Latent Variable Interpretation in Sum-Product Networks", 2016

Bayesian Parameter Learning

Bayesian Learning starts by expressing a prior $p(\mathbf{w})$ over the weights

$\Longrightarrow$ *learning corresponds to computing the posterior based on the data*

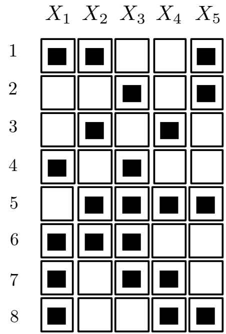
$$p(\mathbf{w}|\mathcal{D}) \propto p(\mathbf{w})p(\mathcal{D}|\mathbf{w})$$

- Moment matching (oBMM) *[Rashwan et al. 2016]*
- oBMM extended with Gaussian distributions *[Jaini et al. 2016]*
- collapsed variational inference algorithm *[Zhao et al. 2016b]*

Structure learning

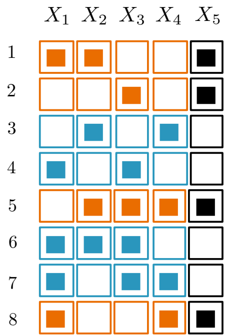
- ***greedy top-down***: LearnSPN and variants
- ***hill climbing***: LearnPSDD and variants
- ***random structures***: RAT-SPNs, XCNets, ...
- ***ensembles*** of circuits: EM, bagging, boosting,...

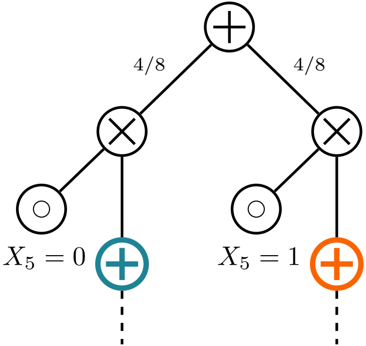
LearnCNet



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

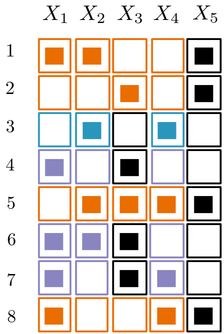
LearnCNet

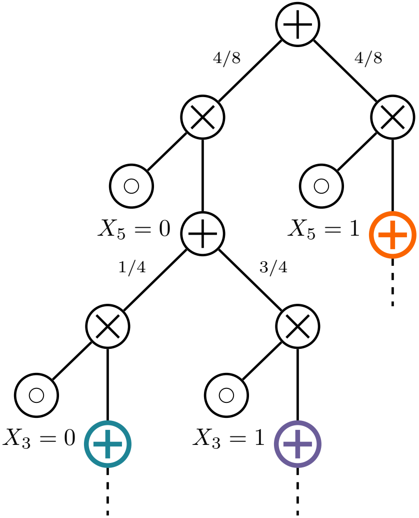




Di Mauro et al., "Learning Accurate Cutset Networks by Exploiting Decomposability", 2015

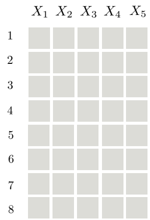
LearnCNet





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

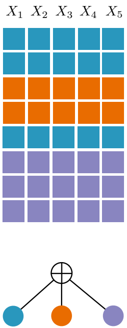
LearnSPN



Learning both structure and parameters of a circuit by starting from a data matrix

Gens et al., "Learning the Structure of Sum-Product Networks", 2013

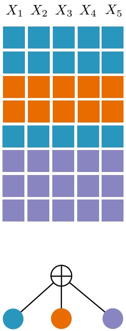
LearnSPN

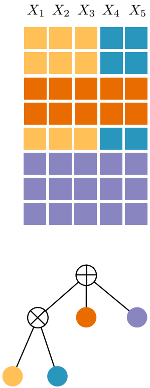


Looking for sub-population in the data—***clustering***—to introduce sum nodes…

Gens et al., "Learning the Structure of Sum-Product Networks", 2013

LearnSPN

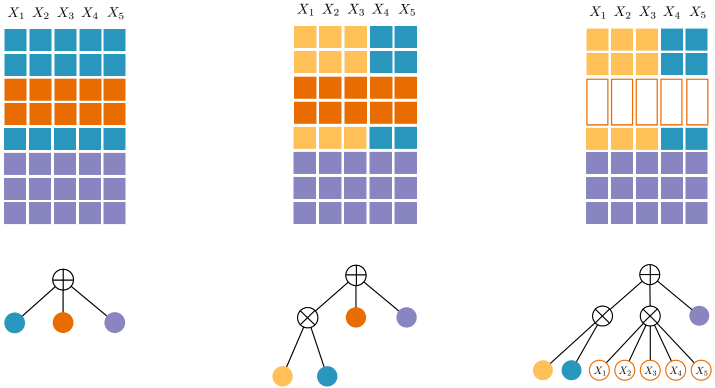




...***seeking independencies among sets of RVs*** to factorize into product nodes

Gens et al., "Learning the Structure of Sum-Product Networks", 2013

LearnSPN



…learning smaller estimators as a ***a recursive data crawler***

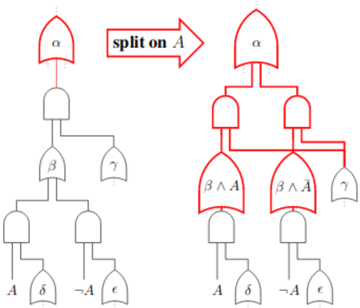
Gens et al., "Learning the Structure of Sum-Product Networks", 2013

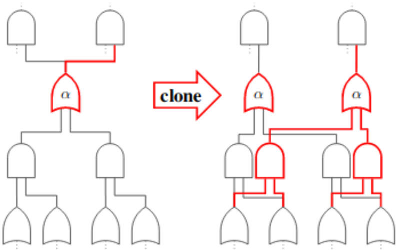
LearnSPN variants

- **ID-SPN** *[Rooshenas et al. 2014]*
- **LearnSPN-b/T/B** *[Vergari et al. 2015]*
- for **heterogeneous data** *[Bueff et al. 2018; 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]*

LearnPSDD

Vtree learning + hill climbing





- local search (split /clone) to maximise a penalized likelihood score

---

Liang et al., "Learning the structure of probabilistic sentential decision diagrams", 2017

Randomized structure learning

Random Tensorized SPNs (RAT-SPNs) *[Peharz et al. 2018]*

- SPNs are obtained by first constructing a random region graph
- subsequently populating the region graph with tensors of SPN nodes
- discriminative+generative parameter learning (SGD/EM + dropout)

Extremely Randomized CNets (XCNets) *[Di Mauro et al. 2017]*

- top-down random conditioning
- learning Chow-Liu trees at the leaves

Ensembles of probabilistic circuits

Single circuits might be not accurate enough or **overfit** training data...

Solution: *ensembles of circuits*!

$\Longrightarrow$ *non-deterministic mixture models: another sum node!*

$$p(\mathbf{X}) = \sum_{i=1}^{K} \lambda_i \mathcal{C}_i(\mathbf{X}), \quad \lambda_i \geq 0 \quad \sum_{i=1}^{K} \lambda_i = 1$$

Ensemble weights and components can be learned separately or jointly

- EM or structural EM
- bagging
- boosting

Bagging

- more efficient than EM
- mixture coefficients are set equally probable
- mixture components can be learned independently on different ***bootstraps***

Adding **random subspace projection** to bagged networks (like for CNets)

- more efficient than bagging

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

Boosting

Boosting Probabilistic Circuits

- BDE: boosting density estimation
  - sequentially grows the ensemble, adding a weak base learner at each stage
  - at each boosting step m, find a weak learner c_m and a coefficient η_m maximizing the weighted LL of the new model

$$f_m = (1 - \eta_m) f_{m-1} + \eta_m c_m$$

- GBDE: a kernel based generalization of BDE—AdaBoost style algorithm
- sequential EM
  - at each step m, jointly optimize η_m and c_m keeping f_{m-1} fixed

Rahman et al., "Learning Ensembles of Cutset Networks", 2016

Applications

Read more in online slides about ...

Applications:

1. *How to compile other models to circuits?*

   $\Longrightarrow$ *PGM compilation, probabilistic databases, probabilistic programming*

2. what have probabilistic circuits been used for?

   $\Longrightarrow$ *computer vision, sop, speech, planning, ...*

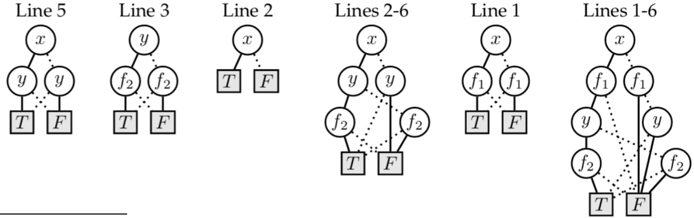
3. what are the current trends and challenges?

   $\Longrightarrow$ *hybrid models, benchmarks, scaling, reasoning*

See: `http://starai.cs.ucla.edu/slides/TPMTutorialUAI19.pdf`

Probabilistic programming

```
1  x = flip(θ1);
2  if(x) {
3    y = flip(θ2)
4  } else {
5    y = x
6  }
```

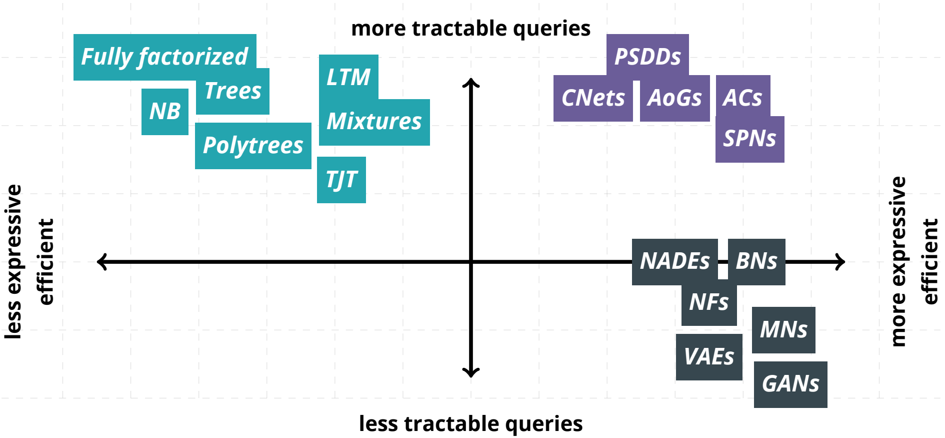


Chavira et al., "Compiling relational Bayesian networks for exact inference", 2006
Holtzen et al., "Symbolic Exact Inference for Discrete Probabilistic Programs", 2019
De Raedt et al.; Riguzzi; Fierens et al.; Vlasselaer et al., "ProbLog: A Probabilistic Prolog and Its Application in Link Discovery."; "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

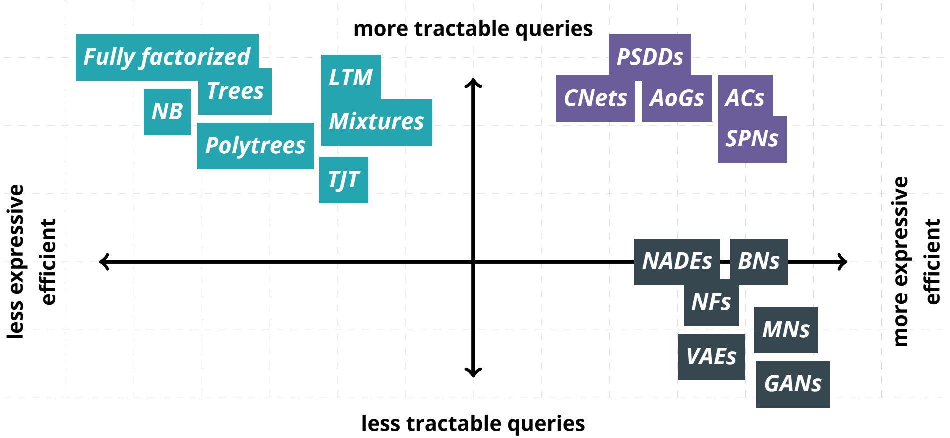
The Logical Conclusions

- Logical roots of probabilistic circuits
- Probabilistic circuits bridge between logic and deep learning
- Bring back world models!
- Powerful general reasoning tool

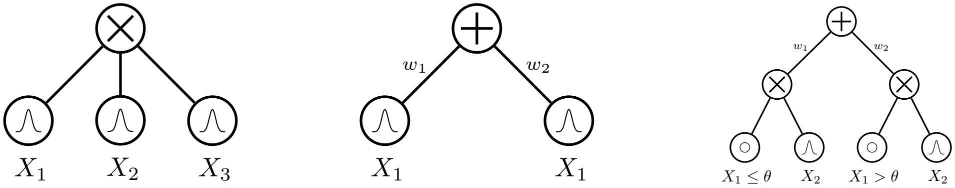
  $\Rightarrow$ *for example in probabilistic programming*
- Elegant knowledge representation formalism



takeaway #1 tractability is a spectrum



takeaway #2: you can be both tractable and expressive



takeaway #3: probabilistic circuits are a foundation for tractable inference and learning

Code

We will soon release **Juice** v0.1: *The Julia Circuit Empanada*

- Learning probabilistic circuits from data and choose to be
  - decomposable – deterministic – structured decomposable
- Evaluate tractable queries
  - EVI – MAR, COND – MAP – Complex queries, expectations, etc.
- Easily compile logical and probabilistic circuits from other representations
- Highly efficient using Julia's SIMD processing capabilities

Tractable Probabilistic Models

Representations
Inference
Learning
Applications

Guy Van den Broeck
University of California, Los Angeles

based on joint AAAI-2020 and UAI-2019 tutorials with

Antonio Vergari
University of California, Los Angeles

YooJung Choi
University of California, Los Angeles

Robert Peharz
TU Eindhoven

Nicola Di Mauro
University of Bari

November 11, 2019 - ***International Spring School on "Uncertainty in AI and data management"*** **- Santiago, Chile**

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