

# subtractive mixture models

# representation, learning & inference

antonio vergari (he/him)



# thanks to...



Lorenzo Loconte *U of Edinburgh* 



Lena Zellinger *U of Edinburgh* 



Aleksanteri Sladek **Aalto U** 



Gennaro Gala **TU Eindhoven** 



Adrian Javaloy **U of Edinburgh** 

and moar...

april-tools.github.io

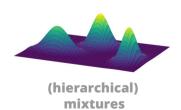
autonomous & provably reliable intelligent learners

about probabilities integrals & logic

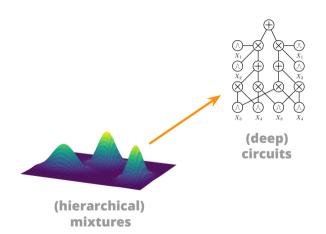
april is probably a recursive identifier of a lab

# today's topic...

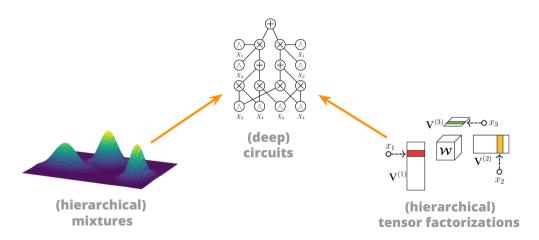
# swiss-army knife of prob ML

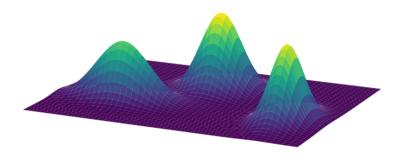


# generalizing them as computational graphs

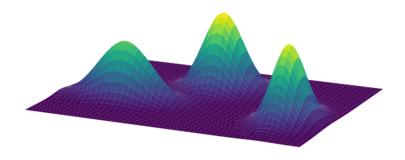


# a single formalism for many models





### who knows mixture models?



### who loves mixture models?

#### Hierarchical Gaussian Mixture Model Splatting for Efficient and Part Controllable 3D Generation

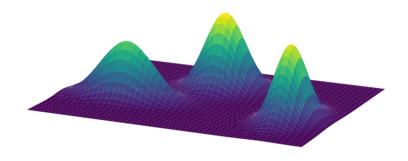
Qitong Yang, Mingtao Feng, Zijie Wu, Weisheng Dong, Fangfang Wu, Yaonan Wang, Ajmal Mian; Proceedings of the Computer Vision and Pattern Recognition Conference (CVPR), 2025, pp. 11104-11114 Inversion of nitrogen and phosphorus contents in cotton leaves based on the Gaussian mixture model and differences in hyperspectral features of UAV

<u>Lei Peng ⊠ , Hui-Nan Xin ⊠ , Cai-Xia Lv ⊠ ,</u> Na Li 题 , <u>Yong-Fu Li 题 , Qing-Long Geng 오 ⊠ ,</u> Shu-Huang Chen ⊠ , Ning Lai 题

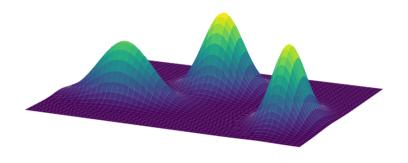
#### **Gaussian Mixture Flow Matching Models**

Hansheng Chen <sup>1</sup> Kai Zhang <sup>2</sup> Hao Tan <sup>2</sup> Zexiang Xu <sup>3</sup> Fujun Luan <sup>2</sup> Leonidas Guibas <sup>1</sup> Gordon Wetzstein <sup>1</sup> Sai Bi <sup>2</sup>

# mixture models are everywhere (still in 2025)



$$c(\mathbf{X}) = \sum_{i=1}^{K} w_i c_i(\mathbf{X}), \quad \text{with} \quad w_i \ge 0, \quad \sum_{i=1}^{K} w_i = 1$$



$$c(\mathbf{X}) = \sum_{i=1}^{K} w_i c_i(\mathbf{X}), \quad \text{with} \quad \frac{\mathbf{w_i} \ge \mathbf{0}}{\sum_{i=1}^{K} w_i} = 1$$

$$\int \sum_{i} w_{i} p_{i}(\mathbf{x}) d\mathbf{x} = \sum_{i} w_{i} \int p_{i}(\mathbf{x}) d\mathbf{x}$$

# mixture models can enable tractable inference

(if components are tractable, e.g., for marginals)

#### **Hierarchical Decompositional Mixtures of Variational Autoencoders**

Ping Liang Tan 12 Robert Peharz 1

Mixtures of Laplace Approximations for Improved *Post-Hoc* Uncertainty in Deep Learning

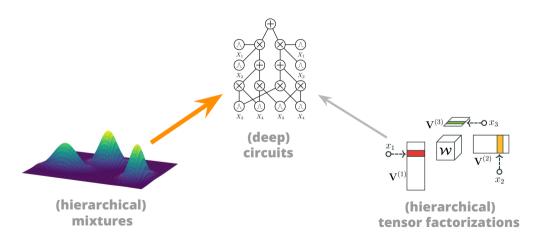
Efficient Mixture Learning in Black-Box Variational Inference

Runa Eschenhagen\*, Erik Daxberger\*, Philipp Hennigi, Agustinus Kristiadi

Alexandra Hotti $^{*123}$  Oskar Kviman $^{*12}$  Ricky Molén $^{12}$  Víctor Elvira $^4$  Jens Lagergren $^{12}$ 

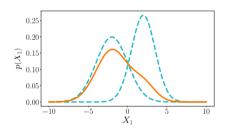
# mixture models can enable tractable inference (even in larger approximate inference pipelines)

# compile mixtures into circuits...



# **GMMs**

#### as computational graphs

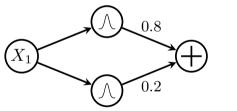


$$p(X_1) = w_1 \cdot p_1(X_1) + w_2 \cdot p_2(X_1)$$





#### as computational graphs



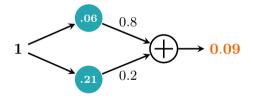
$$p(X_1) = 0.2 \cdot p_1(X_1) + 0.8 \cdot p_2(X_1)$$



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



#### as computational graphs

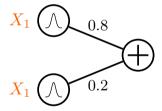


$$p(X_1 = 1) = 0.2 \cdot p_1(X_1 = 1) + 0.8 \cdot p_2(X_1 = 1)$$

⇒ inference = feedforward evaluation



#### as computational graphs



A simplified notation:





# how do we learn them?



## how do we learn them?

 $\Rightarrow$  by maximizing the (log-)likelihood

# which parameters?

how to reparameterize mixtures/circuits

Input distributions.
Sum unit parameters.

# which parameters?

how to reparameterize mixtures/circuits

Input distributions. Each input can be a different parametric distribution

⇒ Bernoullis, Categoricals, Gaussians, exponential families, small NNs, ...

Sum unit parameters.

# which parameters?

how to reparameterize mixtures/circuits

Input distributions. Each input can be a different parametric distribution

**Sum unit parameters.** Enforce them to be non-negative, i.e.,  $w_i \geq 0$  but unnormalized

$$w_i = \exp(\alpha_i), \quad \alpha_i \in \mathbb{R}, \quad i = 1, \dots, K$$

and renormalize the *negative log likelihood* loss

$$\min_{\theta} - \left( \sum_{i=1}^{N} \log \tilde{p}_{\theta}(\mathbf{x}^{(i)}) - \log \int \tilde{p}_{\theta}(\mathbf{x}^{(i)}) d\mathbf{X} \right)$$

or just renormalize the weights, i.e.,  $\sum_i w_i = 1$ 

$$\mathbf{w} = \mathsf{softmax}(\boldsymbol{\alpha}), \quad \boldsymbol{\alpha} \in \mathbb{R}^K$$



## how do we learn them?

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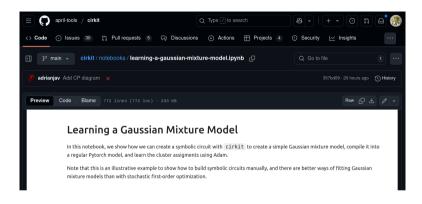
# just SGD your way as usual!

 $\Rightarrow$  or any other gradient-based optimizer



#### learning & reasoning with circuits in pytorch

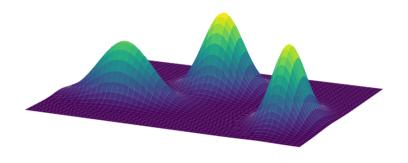
github.com/april-tools/cirkit





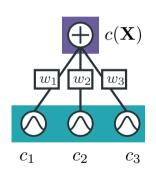
#### a notebook on learning GMMs as circuits

https://github.com/april-tools/cirkit/blob/main/notebooks/ learning-a-gaussian-mixture-model.ipynb



$$c(\mathbf{X}) = \sum_{i=1}^{K} w_i c_i(\mathbf{X}), \quad \text{with} \quad \frac{\mathbf{w_i} \ge \mathbf{0}}{\sum_{i=1}^{K} w_i} = 1$$

are so cool!



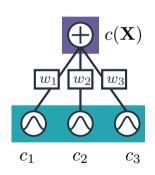
#### easily represented as shallow PCs

these are *monotonic* PCs

if marginals/conditionals are tractable for the components, they are tractable for the MM

they are *universal approximators*...

are so cool!



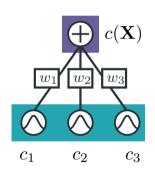
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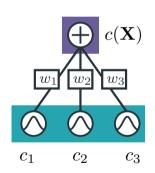
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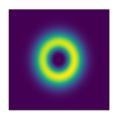


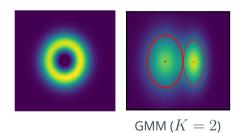
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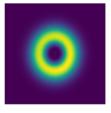
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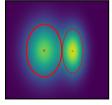
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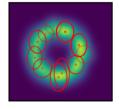


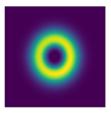
**19**/70

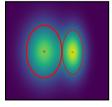




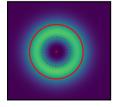










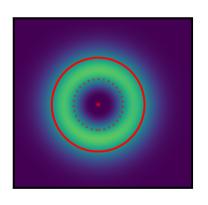


 $\operatorname{GMM}\left(K=2\right) \quad \operatorname{GMM}\left(K=16\right) \quad \operatorname{nGMM}^{2}\left(K=2\right)$ 

# spoiler

shallow mixtures
with negative parameters
can be exponentially more compact than
deep ones with positive parameters

## subtractive MMs



also called negative/signed/subtractive MMs

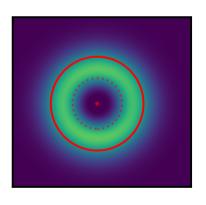


**issue:** how to preserve non-negative outputs?

well understood for simple parametric forms e.g., Weibulls, Gaussians

constraints on variance, mear

## subtractive MMs



also called negative/signed/**subtractive** MMs

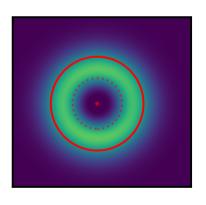
⇒ or non-monotonic circuits,...

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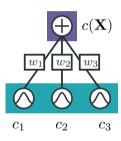
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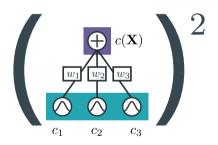
### subtractive MMs as circuits



a **non-monotonic** smooth and (structured) decomposable circuit

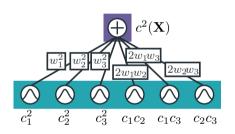
⇒ possibly with negative outputs

$$c(\mathbf{X}) = \sum_{i=1}^{K} w_i c_i(\mathbf{X}), \qquad \mathbf{w_i} \in \mathbb{R},$$

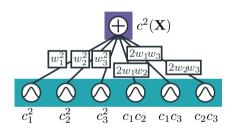


$$c^{2}(\mathbf{X}) = \left(\sum_{i=1}^{K} w_{i} c_{i}(\mathbf{X})\right)^{2}$$

⇒ ensure non-negative output

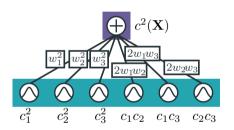


$$c^{2}(\mathbf{X}) = \left(\sum_{i=1}^{K} w_{i} c_{i}(\mathbf{X})\right)^{2}$$
$$= \sum_{i=1}^{K} \sum_{j=1}^{K} w_{i} w_{j} c_{i}(\mathbf{X}) c_{j}(\mathbf{X})$$



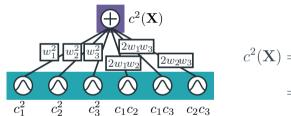
$$c^{2}(\mathbf{X}) = \left(\sum_{i=1}^{K} w_{i} c_{i}(\mathbf{X})\right)^{2}$$
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still a smooth and (str) decomposable PC with  $\mathcal{O}(K^2)$  components!  $\Longrightarrow$  but still  $\mathcal{O}(K)$  parameters



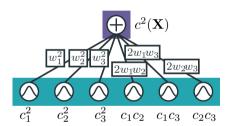
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how to renormalize?



$$c^{2}(\mathbf{X}) = \left(\sum_{i=1}^{K} w_{i} c_{i}(\mathbf{X})\right)^{2}$$
$$= \sum_{i=1}^{K} \sum_{j=1}^{K} w_{i} w_{j} c_{i}(\mathbf{X}) c_{j}(\mathbf{X})$$

to **renormalize**, we have to compute  $\sum_i \sum_j w_i w_j \int c_i(\mathbf{x}) c_j(\mathbf{x}) d\mathbf{x}$ 



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to **renormalize**, we have to compute  $\sum_i \sum_j w_i w_j \int c_i(\mathbf{x}) c_j(\mathbf{x}) d\mathbf{x}$   $\implies$  closed-form for e.g., if  $c_i, c_j$  are **exponential families...!** 



## how do we learn them?



## how do we learn them?

 $\Rightarrow$  by maximizing the (log-)likelihood

# which parameters?

how to reparameterize non-monotonic mixtures/circuits

Input functions.
Sum unit parameters.

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**Input functions.** Each input can be a different parametric *function* 

⇒ Bernoullis, Categoricals, Gaussians, **polynomials**, small NNs, ...

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how to reparameterize non-monotonic mixtures/circuits

**Input functions.** Each input can be a different parametric *function* 

**Sum unit parameters.** They can be negative, i.e.,  $w_i \in \mathbb{R}$  and we we need to renormalize the **negative log likelihood** loss after squaring

$$\min_{\theta} - \left( \sum_{i=1}^{N} 2 \log c_{\theta}(\mathbf{x}^{(i)}) - \log \int c_{\theta}^{2}(\mathbf{x}^{(i)}) d\mathbf{X} \right)$$



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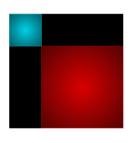
# just SGD your way as usual!

 $\Rightarrow$  or any other gradient-based optimizer

# what about deep mixtures/circuits?

# **GMMs**

### as computational graphs



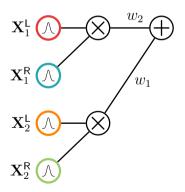


$$p(\mathbf{X}) = w_1 \cdot p_1(\mathbf{X}') \cdot p_1(\mathbf{X}'') + w_2 \cdot p_2(\mathbf{X}''') \cdot p_2(\mathbf{X}'''')$$

⇒ local factorizations...

# **GMMs**

### as computational graphs



$$p(\mathbf{X}) = w_1 \cdot p_1(\mathbf{X}') \cdot p_1(\mathbf{X}'') + w_2 \cdot p_2(\mathbf{X}'''') \cdot p_2(\mathbf{X}'''')$$

⇒ ...are product units

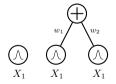
a grammar for tractable computational graphs

I. A simple tractable function is a circuit
 ⇒ e.g., a multivariate Gaussian or small
 neural network



a grammar for tractable computational graphs

- I. A simple tractable function is a circuit
- II. A weighted combination of circuits is a circuit

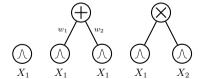


a grammar for tractable computational graphs

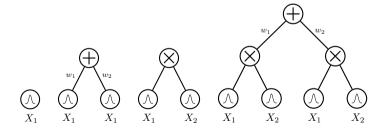
I. A simple tractable function is a circuit

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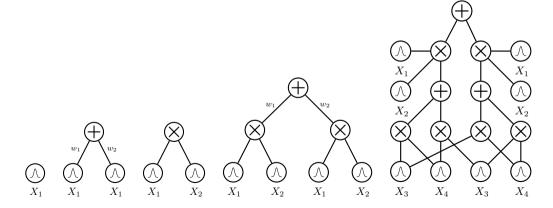
III. A product of circuits is a circuit



a grammar for tractable computational graphs

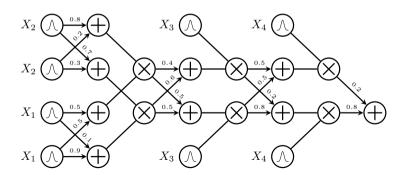


a grammar for tractable computational graphs



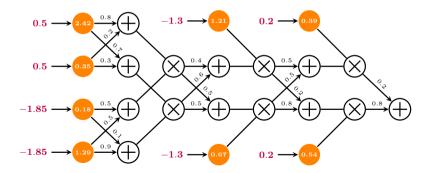
# probabilistic queries = feedforward evaluation

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



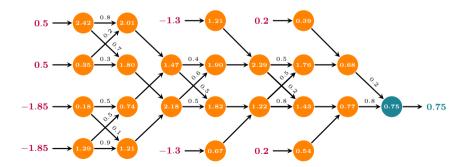
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# probabilistic queries = feedforward evaluation

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



a tensorized definition

I. A set of tractable functions is a circuit layer



a tensorized definition

I. A set of tractable functions is a circuit layerII. A linear projection of a layer is a circuit layer

$$c(\mathbf{x}) = \mathbf{W} \boldsymbol{l}(\mathbf{x})$$





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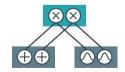
a tensorized definition

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$$c(\mathbf{x}) = \boldsymbol{l}(\mathbf{x}) \odot \boldsymbol{r}(\mathbf{x})$$
 // Hadamard







#### a tensorized definition

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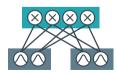
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 // Kronecker









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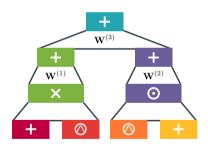








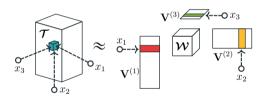
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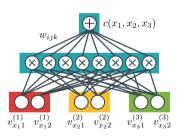


I. A set of tractable functions is a circuit layer
II. A linear projection of a layer is a circuit layer
III. The product of two layers is a circuit layer
stack layers to build a deep circuit!

### tensor factorizations

as circuits





Loconte et al., "What is the Relationship between Tensor Factorizations and Circuits (and How Can We Exploit it)?", TMLR, 2025



#### learning & reasoning with circuits in pytorch

github.com/april-tools/cirkit

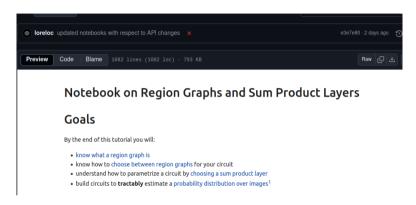




#### a notebook on learning a deep circuit on MNIST

https://github.com/april-tools/cirkit/blob/main/notebooks/ learning-a-circuit.ipynb

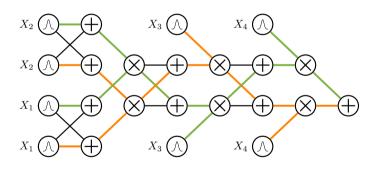




#### mix& match your structure and layers

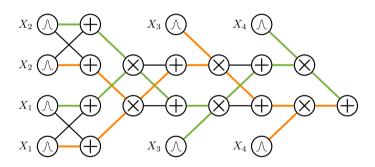
https://github.com/april-tools/cirkit/blob/main/notebooks/ region-graphs-and-parametrisation.ipynb

## deep mixtures



$$p(\mathbf{x}) = \sum_{\mathcal{T}} \left( \prod_{w_j \in \mathbf{w}_{\mathcal{T}}} w_j \right) \prod_{l \in \mathsf{leaves}(\mathcal{T})} p_l(\mathbf{x})$$

## deep mixtures



an exponential number of mixture components!

# ...why PCs?

#### 1. A grammar for tractable models

One formalism to represent many probabilistic models

⇒ #HMMs #Trees #XGBoost, Tensor Networks, ...

# ...why PCs?

#### 1. A grammar for tractable models

One formalism to represent many probabilistic models

⇒ #HMMs #Trees #XGBoost, Tensor Networks, ...

#### 2. Tractability == structural properties!!!

Exact computations of reasoning tasks are certified by guaranteeing certain structural properties. #marginals #expectations #MAP, #product ...

smoothness

decomposability

compatibility

determinism

the combination of certain structural properties guarantees tractable computation of certain query classes

**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

property A

property B

property C

property D

the combination of certain structural properties guarantees tractable computation of certain query classes

**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

property A

property B

property C

property D

#### *tractable* computation of *arbitrary integrals*

$$p(\mathbf{y}) = \int p(\mathbf{z}, \mathbf{y}) d\mathbf{Z}, \quad \forall \mathbf{Y} \subseteq \mathbf{X}, \quad \mathbf{Z} = \mathbf{X} \setminus \mathbf{Y}$$

⇒ **sufficient** and **necessary** conditions for a single feedforward evaluation

⇒ tractable partition function

⇒ also any conditional is tractable

**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

smoothness

decomposability

property C

property D

tractable computation of arbitrary integrals

$$p(\mathbf{y}) = \int p(\mathbf{z}, \mathbf{y}) d\mathbf{Z}, \quad \forall \mathbf{Y} \subseteq \mathbf{X}, \quad \mathbf{Z} = \mathbf{X} \setminus \mathbf{Y}$$

sufficient and necessary conditions for a single feedforward evaluation

⇒ tractable partition function

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**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

smoothness

 $smoothness \land decomposability \Longrightarrow multilinearity$ 

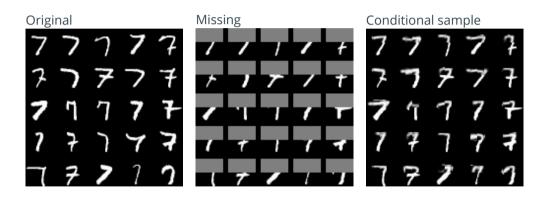
decomposability

property C

property D

**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

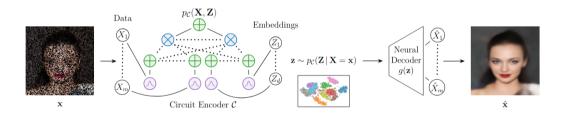
# tractable marginals on PCs



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

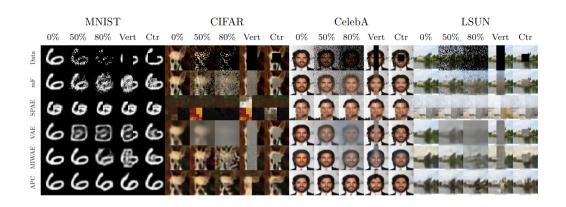
use tractable models inside intractable pipelines where it matters!

#### tractable + intractable



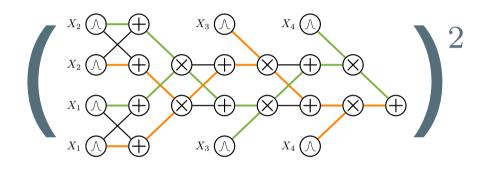
#### tractable conditioning over every missing mask

(under submission)



#### better than (V)AEs for missing values

(under submission)



how to efficiently square (and *renormalize*) a deep PC?

#### compositional inference



```
from cirkit.symbolic.functional import integrate, multiply
# create a deep circuit
c = build symbolic circuit('quad-tree-4')
# compute the partition function of c^2
def renormalize(c):
   c2 = multiply(c, c)
   return integrate(c2)
```

smoothness

decomposability

property C

property D

**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

smoothness

decomposability

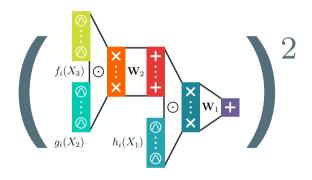
compatibility

property D

Integrals involving two or more functions: e.g., expectations

$$\mathbb{E}_{\mathbf{x} \sim \frac{p}{p}} \left| f(\mathbf{x}) \right| = \int \frac{p(\mathbf{x})}{|f(\mathbf{x})|} d\mathbf{x}$$

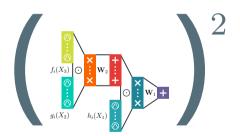
when both  $p(\mathbf{x})$  and  $f(\mathbf{x})$  are circuits



#### how to efficiently square (and *renormalize*) a deep PC?

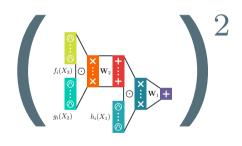
# squaring deep PCs

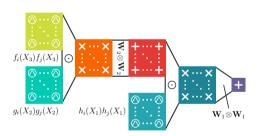
the tensorized way



## squaring deep PCs

the tensorized way

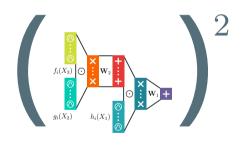


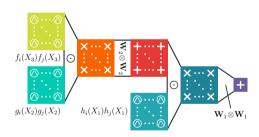


squaring a circuit = squaring layers

## squaring deep PCs

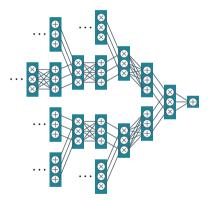
the tensorized way





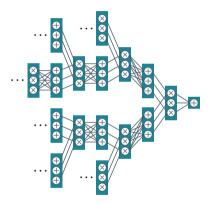
exactly compute  $\int c(\mathbf{x}) c(\mathbf{x}) d\mathbf{X}$  in time  $O(LK^2)$ 

#### theorem I



 $\exists p'$  requiring exponentially large monotonic circuits...

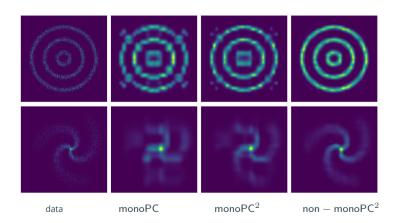
## theorem I



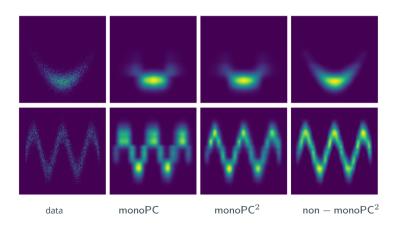
...but compact squared non-monotonic circuits



# more expressive?

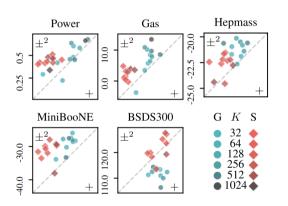


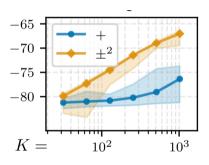
# more expressive?



## how more expressive?

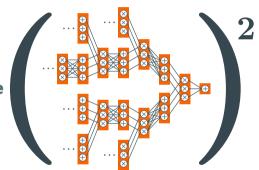
#### real-world data





# theorem II

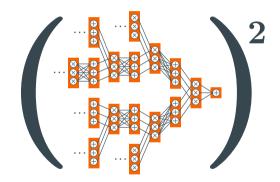
 $\exists \ p''$  requiring exponentially large squared non-mono circuits...

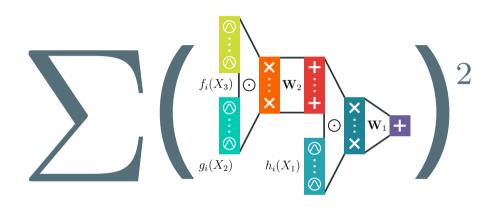


# theorem II



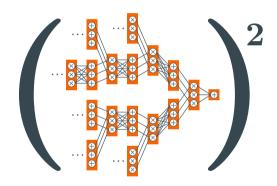
...but compact monotonic circuits...!





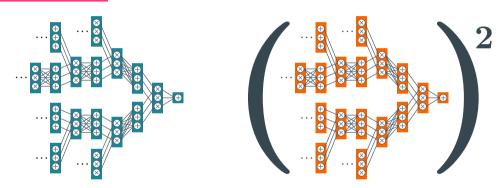
what if we use more that one square?

## theorem III



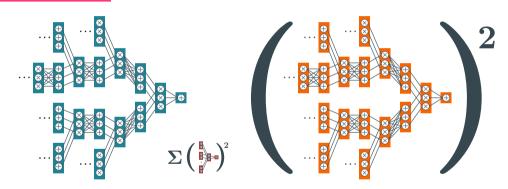
 $\exists p'''$  requiring exponentially large squared non-mono circuits...

# theorem III

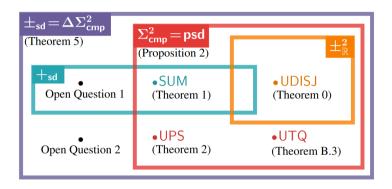


...exponentially large monotonic circuits...

## theorem III



...but compact SOS circuits...!



#### a hierarchy of subtractive mixtures

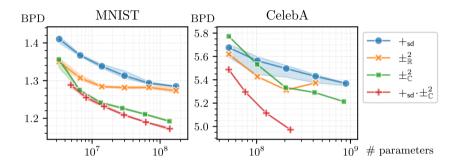
we can define circuits (and hence mixtures) over the Complex:

$$c^2(\mathbf{x}) = c(\mathbf{x})^{\dagger} c(\mathbf{x}), \quad c(\mathbf{x}) \in \mathbb{C}$$

and then we can note that they can be written as a SOS form

$$c^{2}(\mathbf{x}) = r(\mathbf{x})^{2} + i(\mathbf{x})^{2}, \quad r(\mathbf{x}), i(\mathbf{x}) \in \mathbb{R}$$

#### complex circuits are SOS (and scale better!)



complex circuits are SOS (and scale better!)

# takeaway

"use squared mixtures over complex numbers (and you get a SOS for free)"

## takeaway

"use squared mixtures over complex numbers (and you get a SOS for free)"

 $\Rightarrow$  but how to implement them?

### compositional inference



```
from cirkit.symbolic.functional import integrate, multiply,

→ conjugate

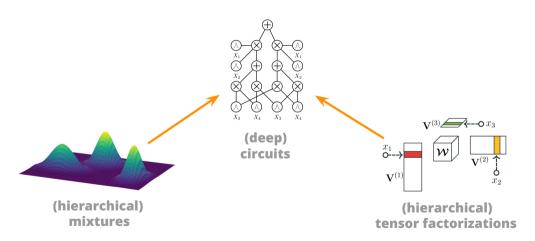
# create a deep circuit with complex parameters
c = build symbolic complex circuit('quad-tree-4')
# compute the partition function of c^2
def renormalize(c):
   c1 = conjugate(c)
   c2 = multiply(c, c1)
   return integrate(c2)
```

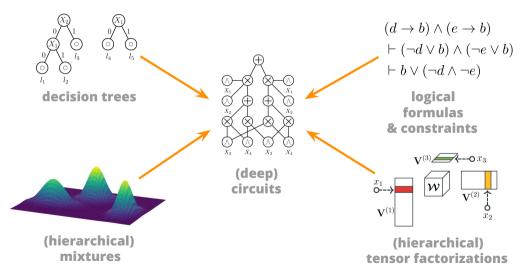


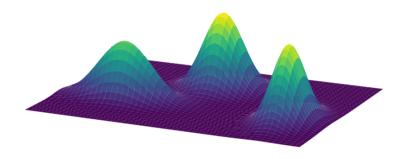
#### a notebook on learning SOS subtractive mixtures

https://github.com/april-tools/cirkit/blob/main/notebooks/ sum-of-squares-circuits.ipynb

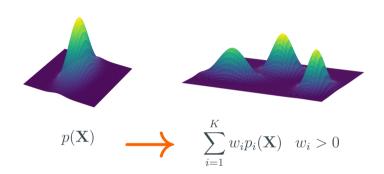
### towards conclusions...

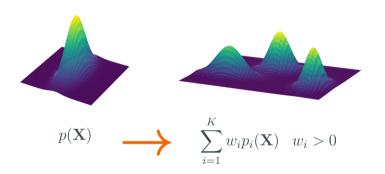






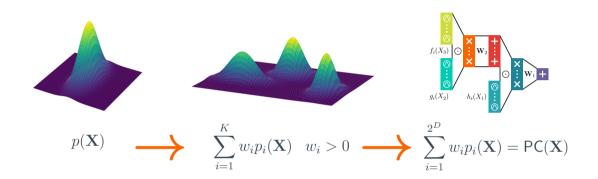
## oh mixtures, you're so fine you blow my mind!

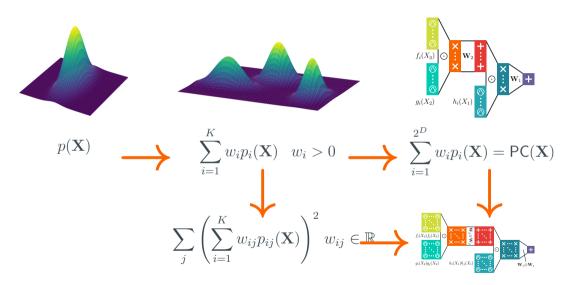




"if someone publishes a paper on **model A**, there will be a paper about **mixtures of A** soon, with high probability"

A. Vergari

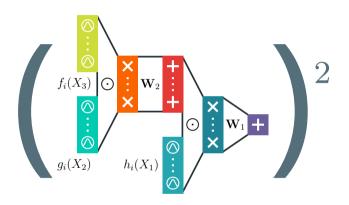






#### learning & reasoning with circuits in pytorch

github.com/april-tools/cirkit



## questions?

### structural properties

smoothness

decomposability

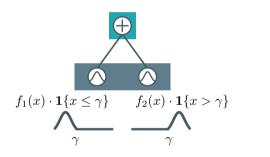
compatibility

determinism

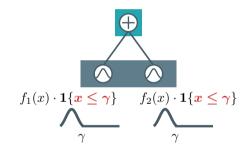
**Vergari** et al., "A Compositional Atlas of Tractable Circuit Operations for Probabilistic Inference", NeurIPS, 2021

### determinism

the inputs of sum units are defined over disjoint supports



deterministic circuit



non-deterministic circuit