Sum of Squares Circuits

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There are many probabilistic models...

Estimate $p(\mathbf{x})$ with a model

GMMs | Trees | PSD | SNFs

HMMs | NTFs | BMs

MAFs | VAEs | GANs

LLMs | Dffusion | EBMs

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Probe $p(\mathbf{x})$ to solve tasks

Lossless data (de-)compression:

$p(x_i \mid x_1, \ldots, x_{i-1})$

Neurosymbolic reasoning:

$\mathbb{E}_{\mathbf{x} \in p(\mathbf{x})}[\kappa(\mathbf{x})] = \int_{\mathcal{X}} p(\mathbf{x})\kappa(\mathbf{x})\mathrm{d}\mathbf{x}$

Liu, Mandt, and Broeck, “Lossless Compression with Probabilistic Circuits”, 2022

Ahmed et al., “Semantic probabilistic layers for neuro-symbolic learning”, 2022

There are many probabilistic models...

Estimate $p(\mathbf{x})$ with a model

Expressive generative models
(often intractable inference)

MAFs | VAEs | GANs

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Models supporting tractability
(often not expressive enough)

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"How to build probabilistic models that are expressive yet support tractable inference?"

Circuits: why?

Neural networks whose **tractability** and **expressiveness** can be analyzed theoretically

Circuits: why?

Neural networks whose **tractability** and **expressiveness** can be analyzed theoretically

Complexity of **exact inference** is polynomial w.r.t. **circuit size**, under structural assumptions

conditionals: $p(x_i \mid x_1, \ldots, x_{i-1})$

expectations: $\mathbb{E}_{\mathbf{x} \in p(\mathbf{x})}[\kappa(\mathbf{x})]$

...and more!

Choi, Vergari, and Broeck, Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling, 2020

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

Circuits: why?

Neural networks whose **tractability** and **expressiveness** can be analyzed theoretically

Framework to study expressiveness,
based on **circuit complexity theory**

Valiant, "Negation can be exponentially powerful", 1979

Colnet and Mengel, "A Compilation of Succinctness Results for Arithmetic Circuits", 2021

Circuits: why?

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Framework to study expressiveness, based on **circuit complexity theory**

GMMs Trees PSD SNFs

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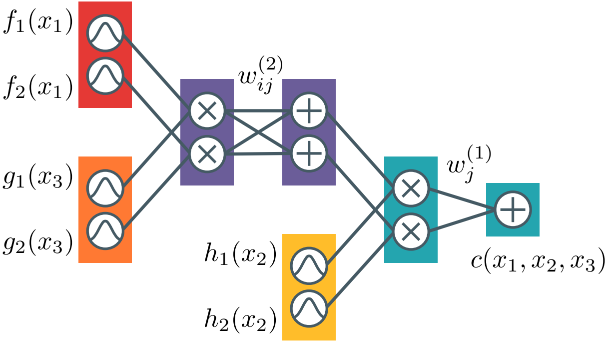
...are all circuits! (more later)

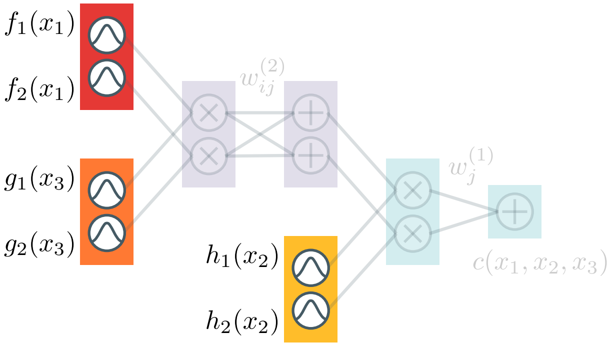
Valiant, “Negation can be exponentially powerful”, 1979

Colnet and Mengel, “A Compilation of Succinctness Results for Arithmetic Circuits”, 2021

Circuits: what?



Circuits: what?



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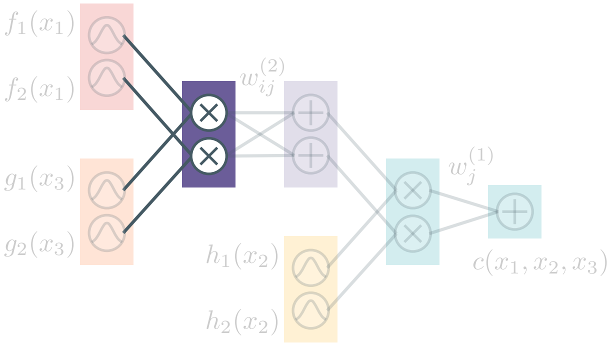

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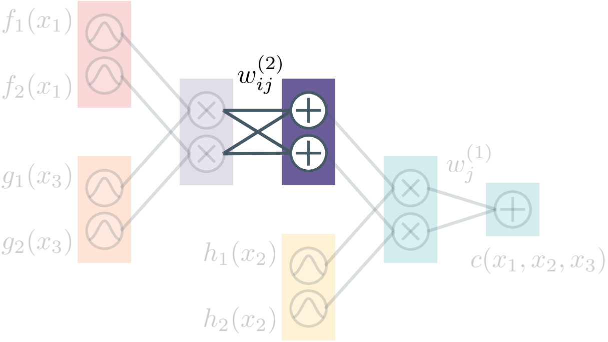

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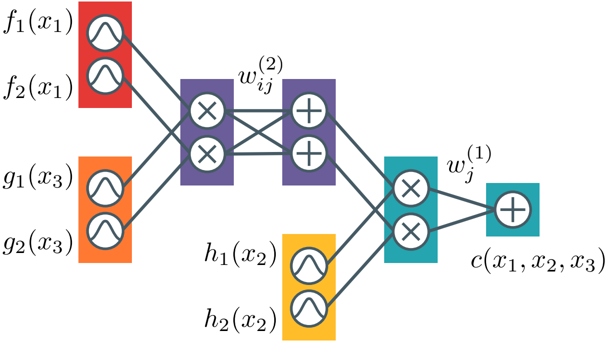

Circuits: how to model distributions?

Monotonic circuits

$$p(\mathbf{x}) = \frac{1}{Z}\, c(\mathbf{x}), \quad c(\mathbf{x}) \geq 0$$

where parameters and input functions are **positive**

Choi, Vergari, and Broeck, Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Modeling, 2020

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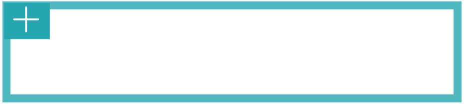
 $=$ set of distributions modeled by **polysize** circuits

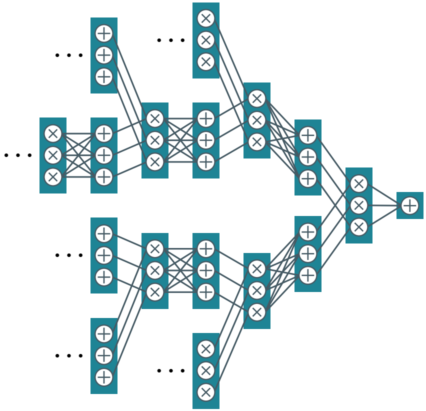


A limitation of monotonic circuits

 = set of distributions modeled by **polysize** circuits

- UDISJ

Loconte et al., "Subtractive Mixture Models via Squaring: Representation and Learning", 2024



$\exists\, p$ requiring **exponentially large** **monotonic circuits**...

Loconte et al., "Subtractive Mixture Models via Squaring: Representation and Learning", 2024

Squared circuits

$$p(\mathbf{x}) = \frac{1}{Z}\, c^2(\mathbf{x}), \quad c(\mathbf{x}) \in \mathbb{R}$$

where parameters and input functions can be **negative**

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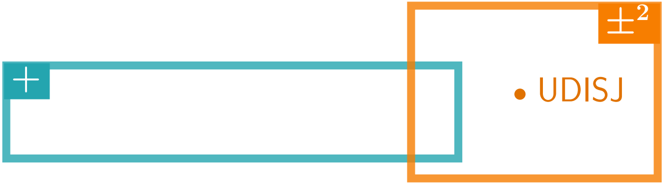

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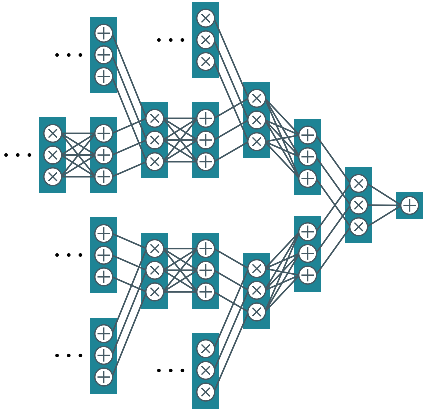
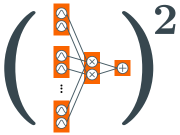
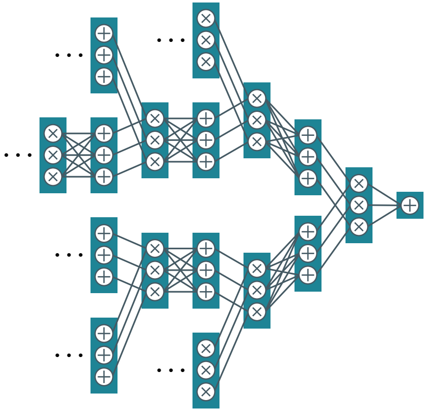
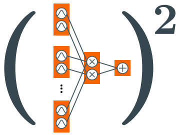




...instead **squared circuits** require **polynomial size**

Loconte et al., "Subtractive Mixture Models via Squaring: Representation and Learning", 2024



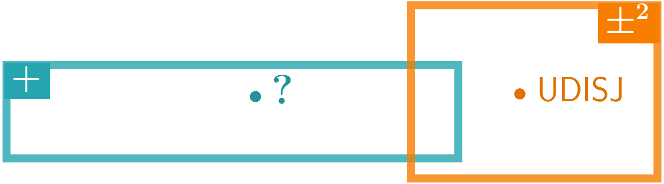


Squared circuits more expressive than **monotonic** ones

Loconte et al., “Subtractive Mixture Models via Squaring: Representation and Learning”, 2024

Outline

1. *Can monotonic circuits be more expressive than squared?*



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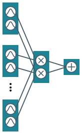
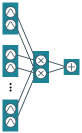
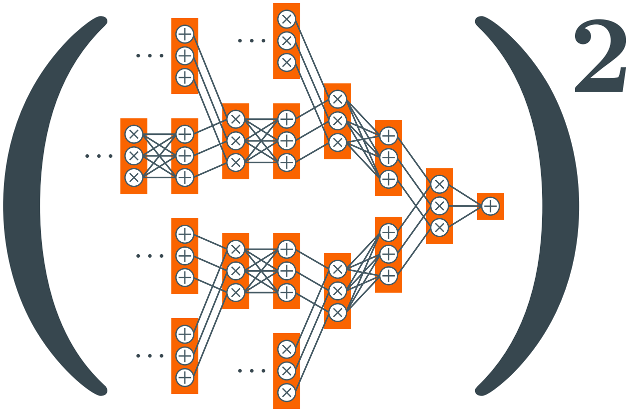


$\exists\, p$ requiring **polysize** **monotonic circuits**...





...but require **exponentially large** **squared circuits**

Theorem 1.

There is a class of non-negative functions $\mathcal{F}$ over $d = k(k+1)$ variables that can be encoded by a PC in $+_{\mathsf{sd}}$ having size $\mathcal{O}(d)$. However, the smallest $c^2 \in \pm^2_{\mathbb{R}}$ computing any $F \in \mathcal{F}$ requires $|c|$ to be at least $2^{\Omega(\sqrt{d})}$.

Squaring alone can reduce expressiveness!

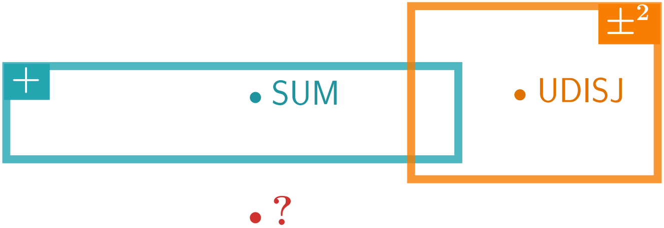
Wang and Van den Broeck, On the Relationship Between Monotone and Squared Probabilistic Circuits, 2024

Outline

1. *Can monotonic circuits be more expressive than squared?*

   $\Longrightarrow$ Yes!

2. *How to build models more expressive than <u>both</u>?*



Sum of squares (SOS) circuits

$p(\mathbf{x}) = \frac{1}{Z}\sum_{i=1}^{r} c_i^2(\mathbf{x}), \quad c_i(\mathbf{x}) \in \mathbb{R}$

where parameters and input functions can be **negative**

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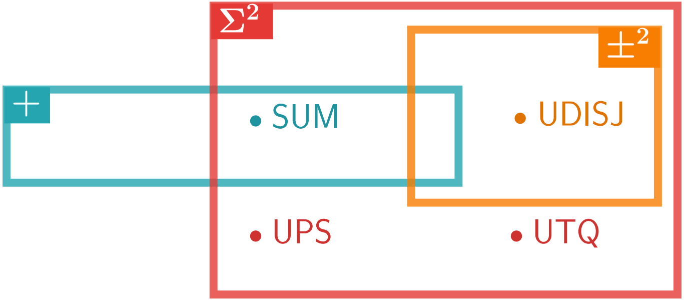
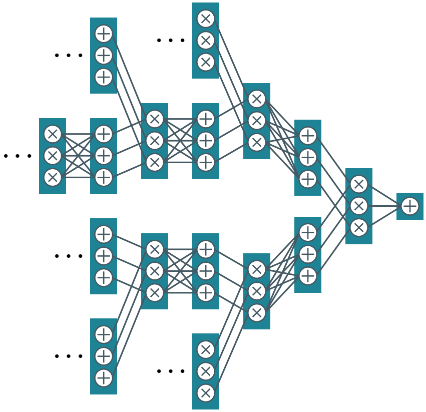
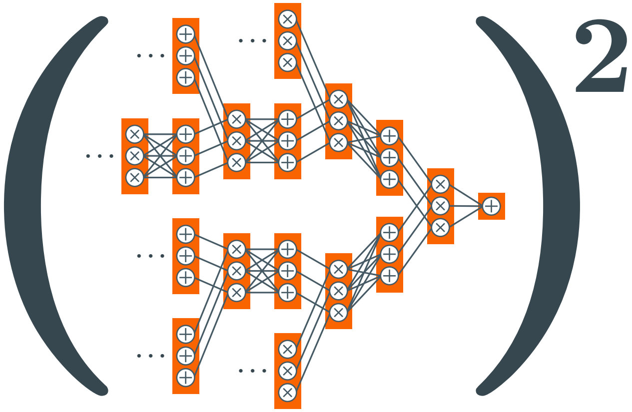
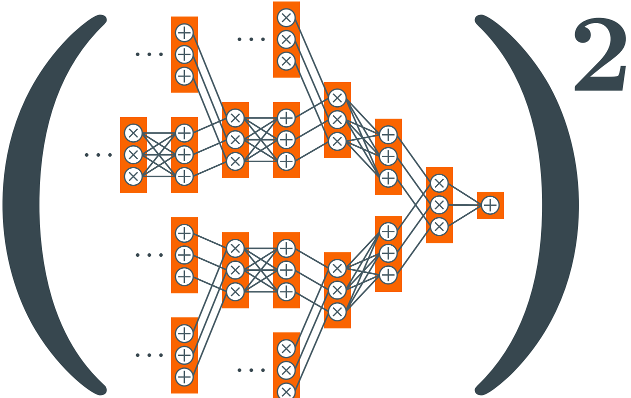


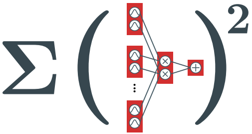


$\exists\, p$ requiring **exponentially large monotonic circuits**...



...and also **exponentially large squared circuits** ...





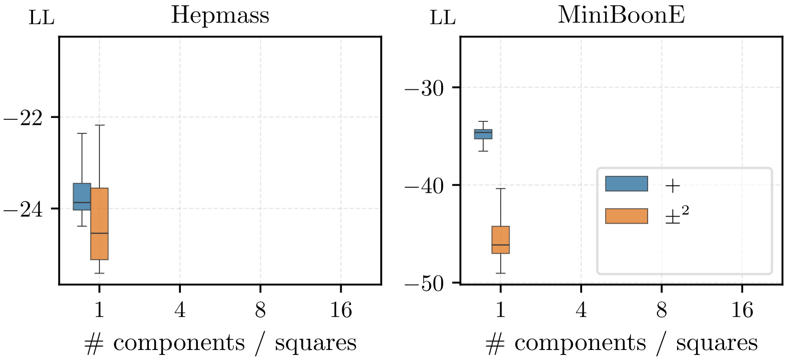
...but a **sum of squares (SOS)** **polysize** circuits

Theorem 2.

There is a class of non-negative functions $\mathcal{F}$ over d variables that can be represented by a PC in $\Sigma^2_{\textsf{cmp}}$ of size $\mathcal{O}(d^3)$. However, (i) the smallest PC in $+_{\textsf{sd}}$ computing any $F \in \mathcal{F}$ has at least size $2^{\Omega(\sqrt{d})}$, and (ii) the smallest $c^2 \in \pm^2_{\mathbb{R}}$ computing F obtained by squaring a structured-decomposable circuit c, requires $|c|$ to be at least $2^{\Omega(\sqrt{d})}$.

SOS can surpass both expressiveness limitations!

Experiments



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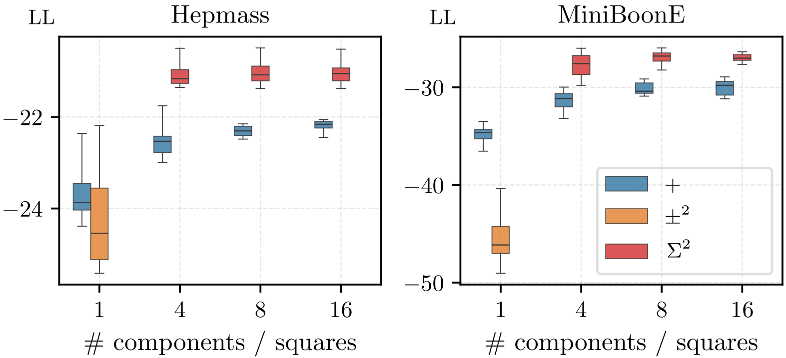

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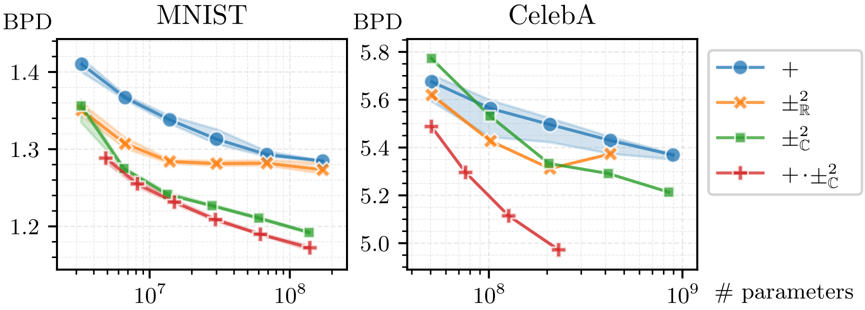

Outline

1. *Can monotonic circuits be more expressive than squared?*

   $\Longrightarrow$ Yes!

2. *How to build models more expressive than <u>both</u>?*

   $\Longrightarrow$ SOS circuits!

3. *How are SOS circuits related to other probabilistic models?*

$$p(\mathbf{x}) \propto \boldsymbol{\kappa}(\mathbf{x})^\top \mathbf{A} \boldsymbol{\kappa}(\mathbf{x})$$

with $\mathbf{A} \in \mathbb{R}^{d \times d}$ PSD

Positive Semi-Definite models

Rudi and Ciliberto, “PSD Representations for Effective Probability Models”, 2021

Tsuchida, Ong, and Sejdinovic, “Squared Neural Families: A New Class of Tractable Density Models”, 2023

Glasser et al., “Expressive power of tensor-network factorizations for probabilistic modeling”, 2019

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$$p(\mathbf{x}) \propto \mu(\mathbf{x}) ||\mathrm{NN}_{\sigma,\Theta}(\boldsymbol{t}(\mathbf{x}))||_2^2$$

Squared Neural Families

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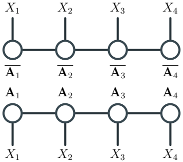

$$p(\mathbf{x}) \propto \psi(\mathbf{x}) \psi(\mathbf{x})^\dagger, \psi(\mathbf{x}) \in \mathbb{C}$$

Complex Born machines

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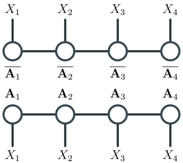

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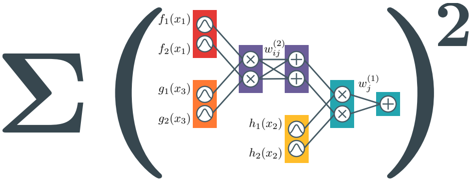

...can be reduced to SOS circuits!

$\implies$ *summing squares boosts expressiveness*

$\implies$ *complex parameters help*

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Takeaways

1. A more precise expressiveness characterization of squared circuits

Paper *Code*

loreloc.github.io

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Takeaways

1. A more precise expressiveness characterization of squared circuits

2. SOS circuits can be more expressive than both monotonic & squared circuits

Paper ***Code***

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Takeaways

1. A more precise expressiveness characterization of squared circuits

2. SOS circuits can be more expressive than both monotonic & squared circuits

3. Connect SOS with other models, thus we understand why they are expressive

Paper ***Code***

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