Probabilistic Flow Circuits: Towards Unified Deep Models for Tractable Probabilistic Inference

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What ?

Motivation

The generative modeling dichotomy: tractability vs. expressivity

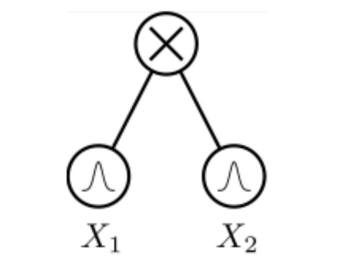
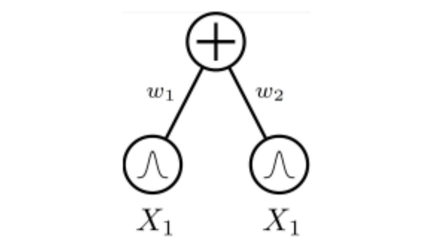
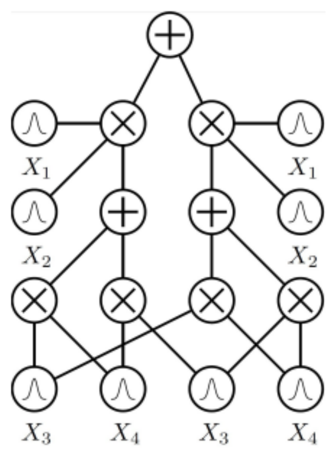
Tractable — **No Free Lunch** — **Expressive**

Naïve Bayes, Trees, And-Or-Graphs, SPN, Einsum Networks, Normalizing Flows, Autoregressive, VAEs, GANS

Can we borrow concepts from both ends of the spectrum to **bridge** this gap? Build **expressive** and **tractable** models?

Background

Tractability with Probabilistic Circuits

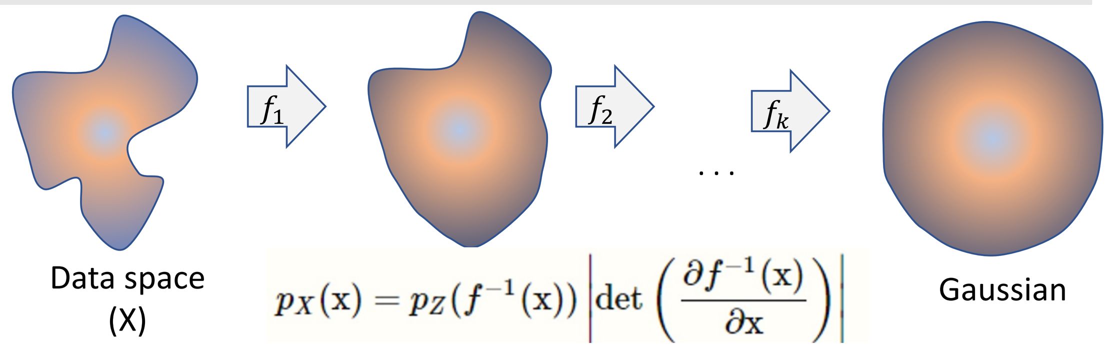
Leaf Nodes	Product Nodes	Sum Nodes	Stacked
	 $p(X_1,X_2)=p(X_1)\cdot p(X_2)$	 $p(X_1)=w_1p_1(X_1)+w_2p_2(X_1)$	
Simple univariate distribution	Represents **factorizations**	Represents **mixtures**	
	Enables tractability	Adds expressivity	

Expressivity with Normalizing Flows

Learn probability distributions using invertible transformations and the change of variables formula

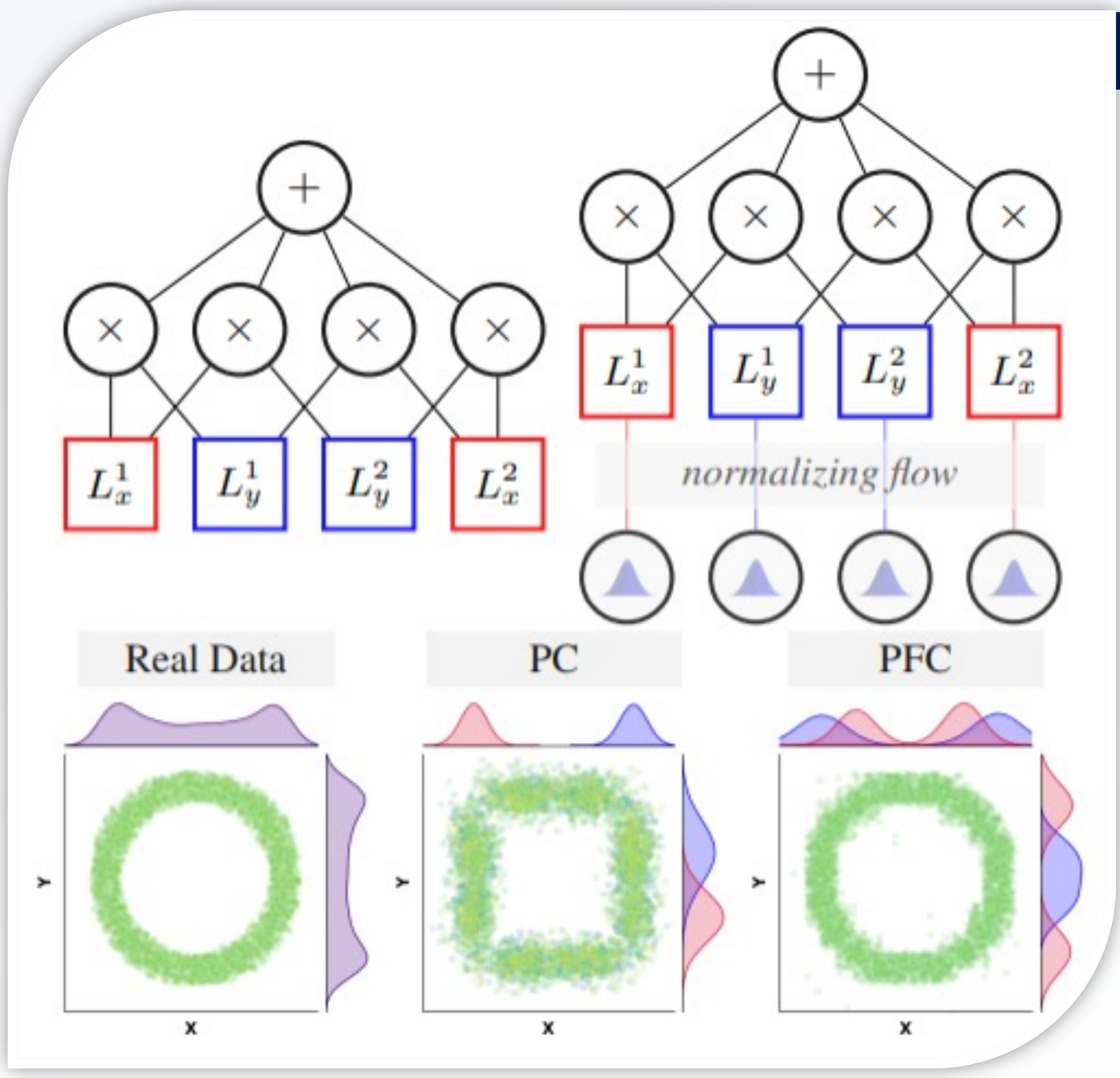
Neural Network parameterization

Supports **exact** density evaluation



$$p_X(x)=p_Z(f^{-1}(x))\left|\det\left(\frac{\partial f^{-1}(x)}{\partial x}\right)\right|$$

How ?



Probabilistic Flow Circuit (PFC)

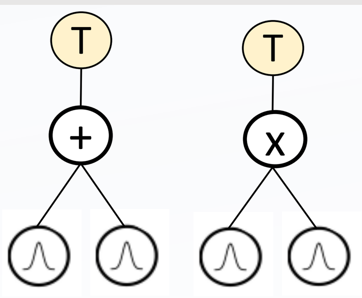
Has added Expressivity	Retains Tractability
Can model arbitrarily complex distributions at the leaves	As it encodes **factorizations** of the joint distribution

Integrating Flows with PCs

Introduce **invertible transform nodes** arbitrarily in a PC [Pevny et. Al 2020]

Represents **normalizing** flows

Adds expressivity



$$T(N(\boldsymbol{x}))=N(f(\boldsymbol{x}))|\det J_f|$$

$N=\{\oplus, \otimes, \bigcirc\}$

But this affects decomposability → Tractability violated → Need more structure

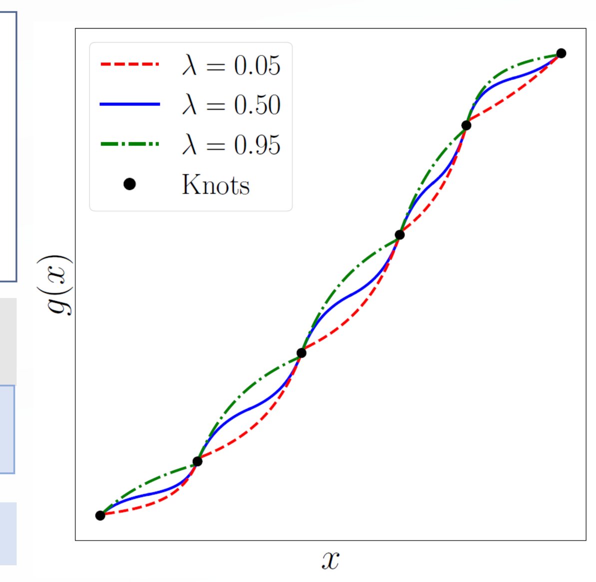
τ-Decomposability

- When defined over a product node, T needs to transform the variables involved in the scope of its children **independently**
- A **necessary condition** for tractability of marginal and conditional

Implications: Reduces to having flows at the **leaves**!

What transformation to use? Linear Rational Splines (LRS)

1. Divide the data space into K bins and fit a polynomial function f_k within each bin
2. Use monotone linear rational functions of the form: $f(x)=\frac{ax+b}{cx+d}$



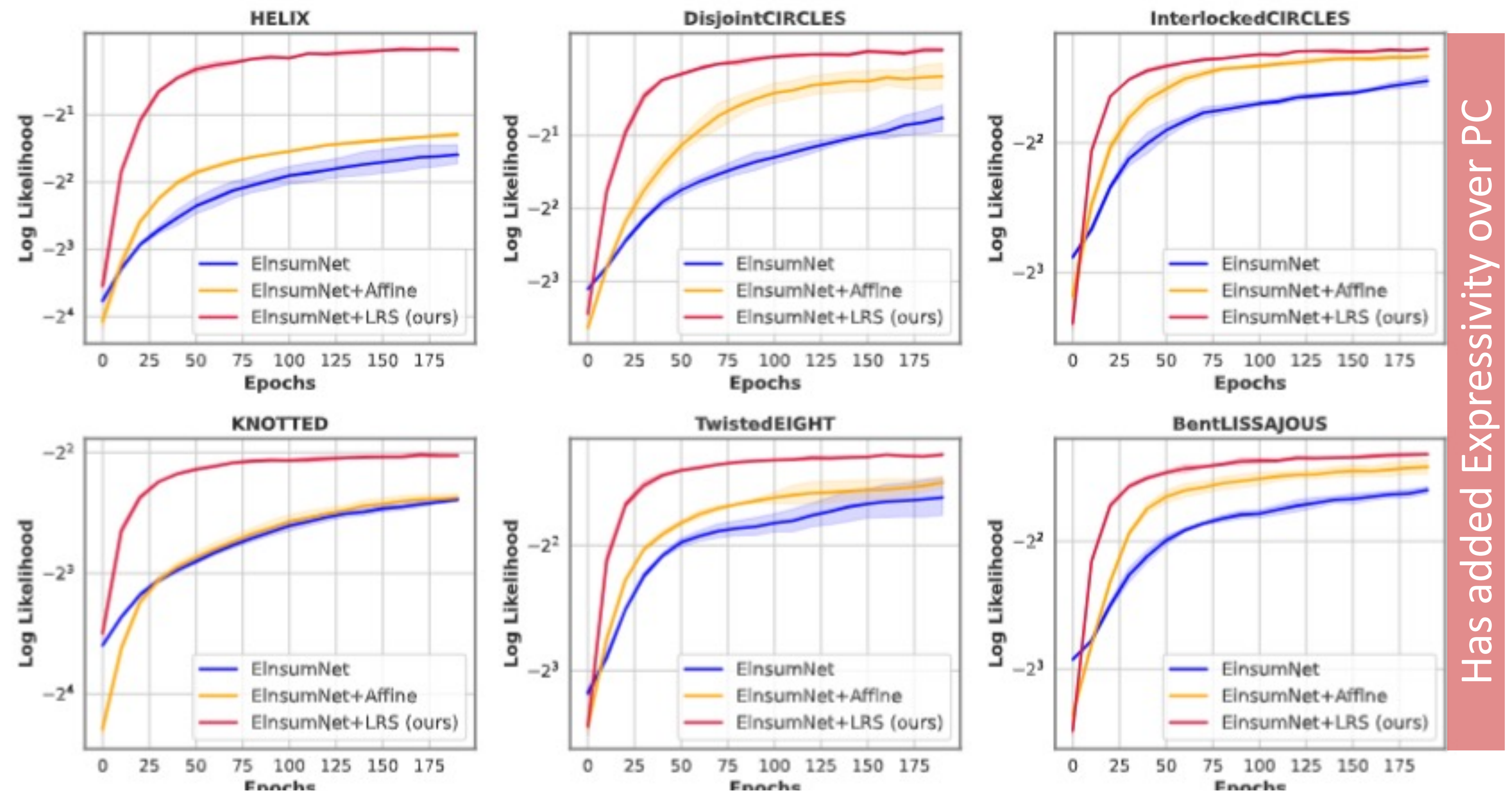
A PFC with LRS transformations is tractable for

Evidential	Marginal	Conditional	MAP

If you use a Student's-t base distribution and PC is deterministic

What do we get ?

Empirical Evaluations



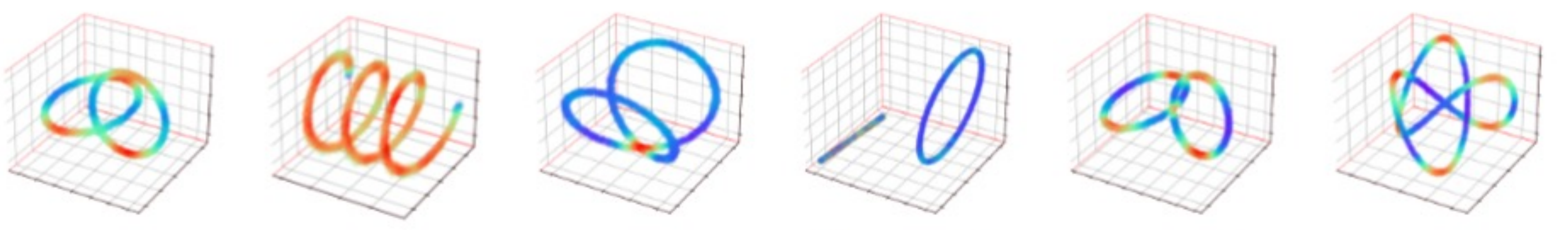
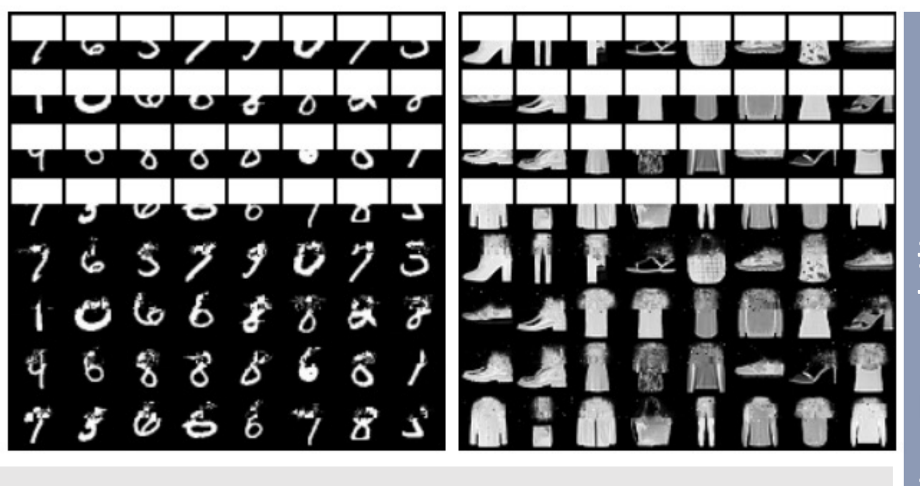
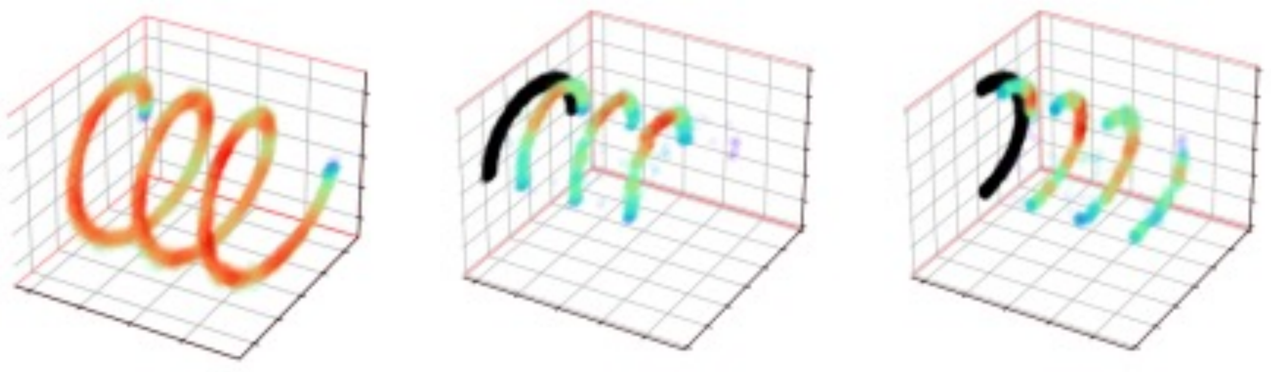


Image Inpainting

Can fill in missing data by sampling from the conditional distribution over occluded pixels



Controlled generation



Retains Tractability

Acknowledgements

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References

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[2.] Pevný, Tomáš, et al. "Sum-product-transform networks: Exploiting symmetries using invertible transformations." PGM 2020.

[3.] Peharz, Robert, et al. "Einsum networks: Fast and scalable learning of tractable probabilistic circuits." ICML 2020.

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