StARLinG LAB
THE UNIVERSITY OF TEXAS AT DALLAS

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TECHNISCHE UNIVERSITÄT DARMSTADT

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

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UTD

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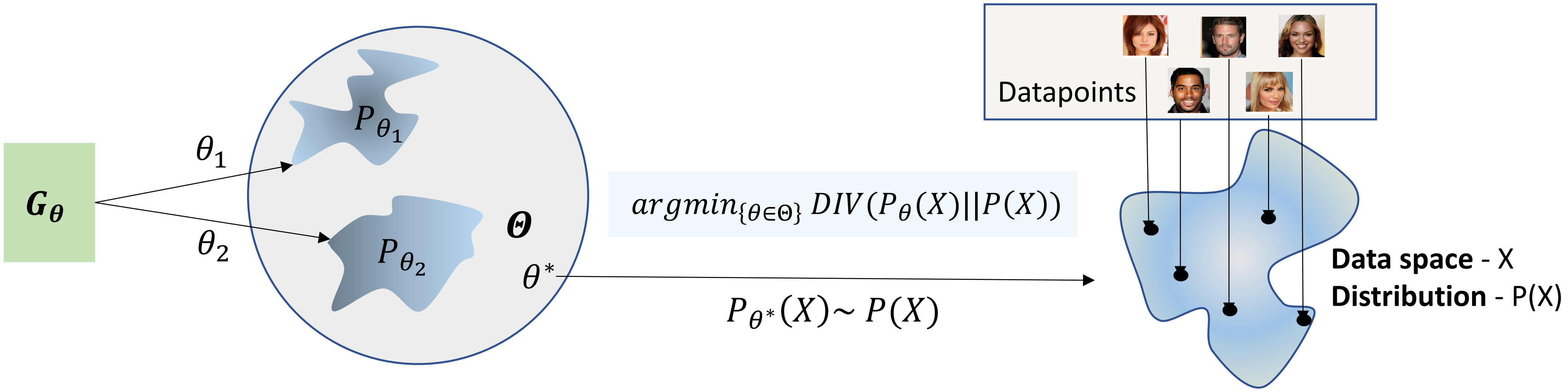
UTD

Motivation

Building Expressive and Tractable Generative Models



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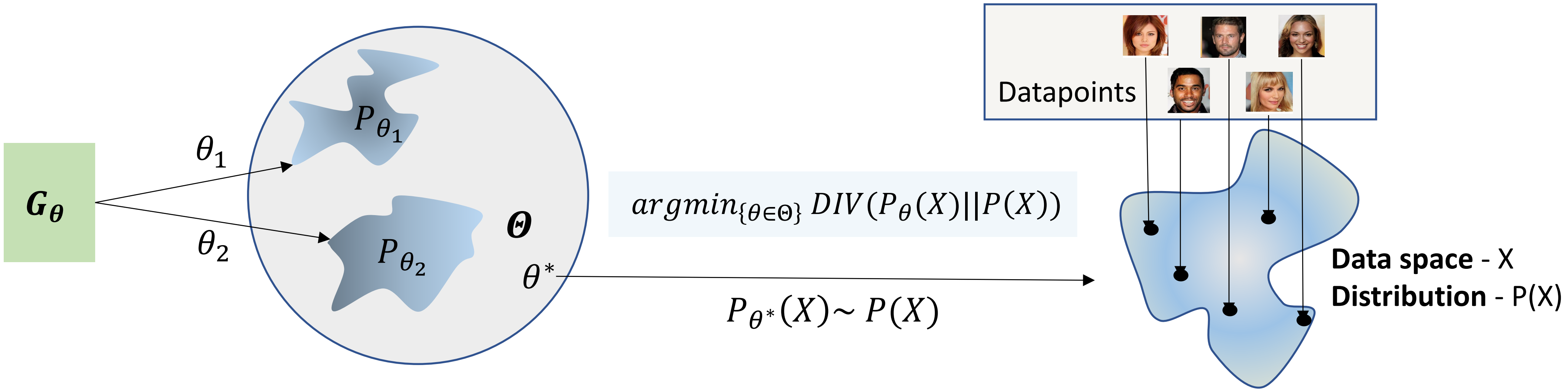

Expressivity	Characterizes the complexity of functions that can be represented. A more expressive model can better approximate complex distributions in high-dimensional spaces

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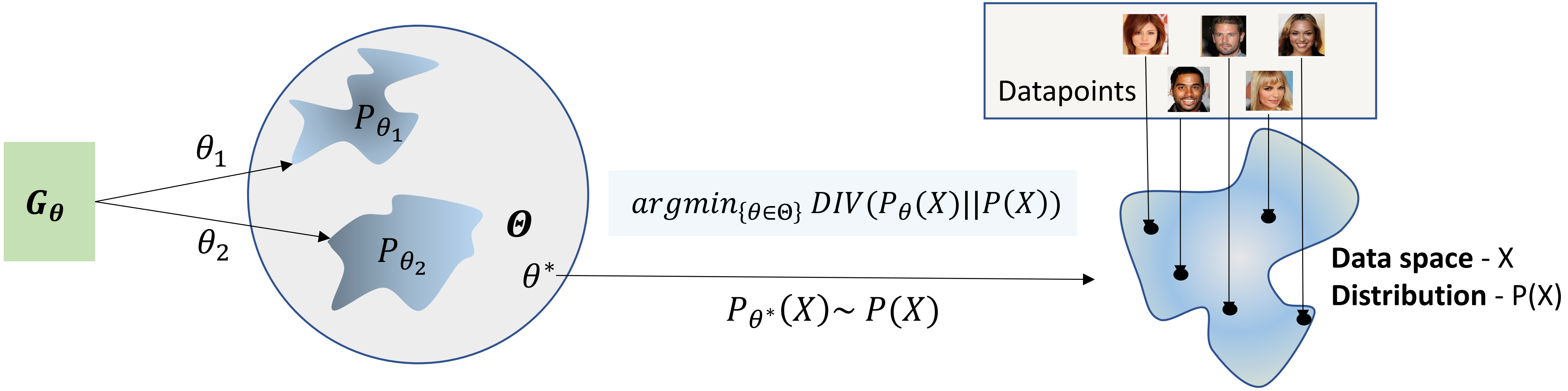
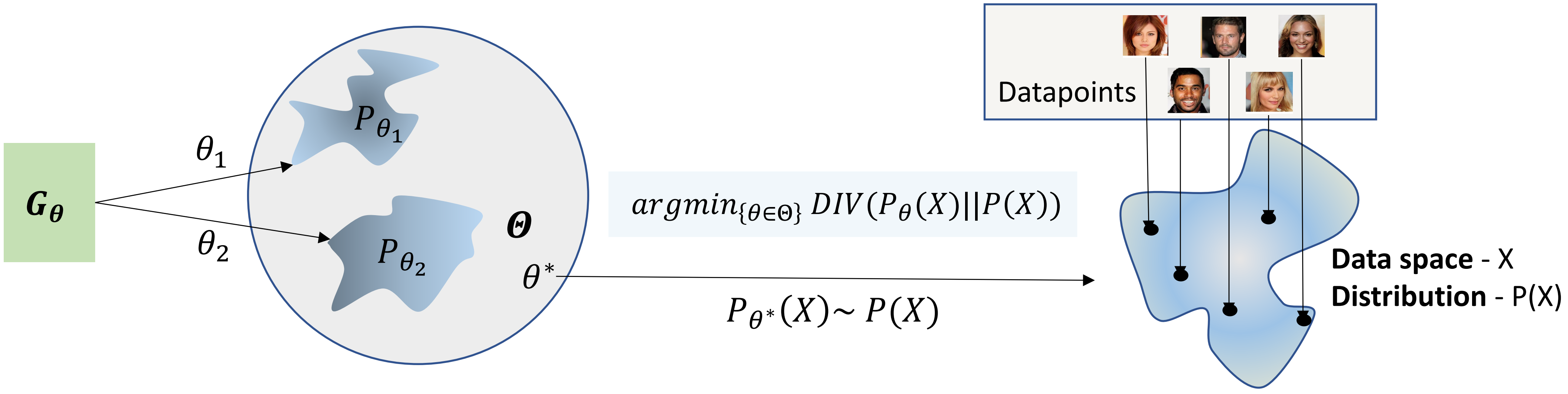


Expressivity	Characterizes the complexity of functions that can be represented. A more expressive model can better approximate complex distributions in high-dimensional spaces
Tractability	Ability to answer probabilistic **inference** queries about the learned distribution in **polynomial** time. Can **reason** probabilistically about the learned distribution.

Motivation

Building Expressive and Tractable Generative Models



Using Normalizing Flows

Expressivity

Characterizes the complexity of functions that can be represented.

A more expressive model can better approximate complex distributions in high-dimensional spaces

Using Probabilistic Circuits

Tractability

Ability to answer probabilistic **inference** queries about the learned distribution in **polynomial** time.

Can **reason** probabilistically about the learned distribution.

Probabilistic Circuits

Hierarchical Mixtures of Simple Factorized Distributions

Computational graphs that recursively define distributions via 3 types of nodes

Probabilistic Circuits

Hierarchical Mixtures of Simple Factorized Distributions

Computational graphs that recursively define distributions via 3 types of nodes

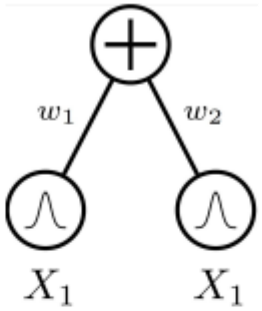
$p(X) = Normal(X)$

Leaf nodes
Simple univariate distributions

Probabilistic Circuits

Hierarchical Mixtures of Simple Factorized Distributions

Computational graphs that recursively define distributions via 3 types of nodes



$p(X) = Normal(X)$

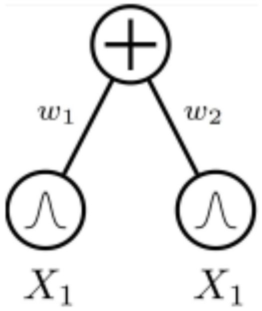
$p(X_1) = w_1 p_1(X_1) + w_2 p_2(X_1)$

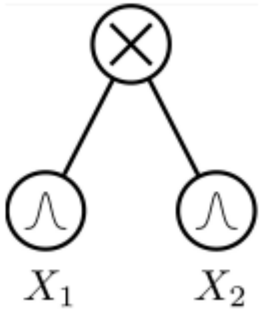
Leaf nodes	Sum nodes
Simple univariate distributions	Represents **mixtures**
	Adds expressivity

Probabilistic Circuits

Hierarchical Mixtures of Simple Factorized Distributions

Computational graphs that recursively define distributions via 3 types of nodes





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

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

Leaf nodes	Sum nodes	Product nodes
Simple univariate distributions	Represents **mixtures**	Represents **factorizations**
	Adds expressivity	Enables tractability

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Hierarchical Mixtures of Simple Factorized Distributions

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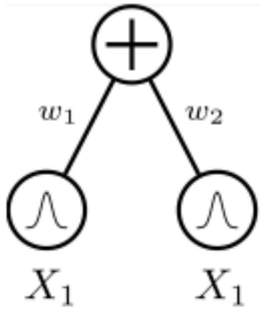

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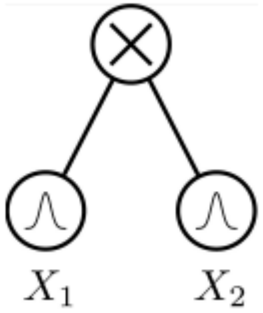
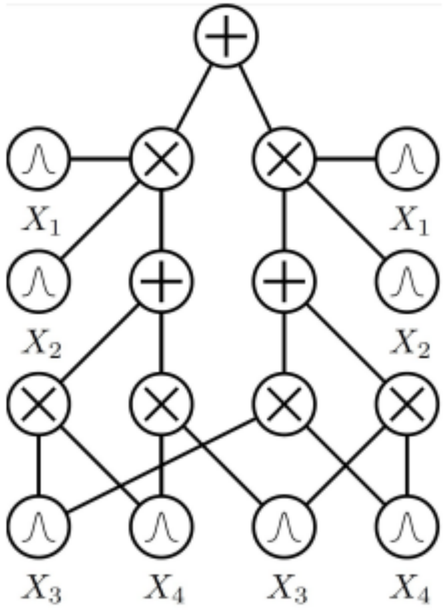
Sum nodes
Represents **mixtures**
Adds expressivity



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

Product nodes
Represents **factorizations**
Enables tractability

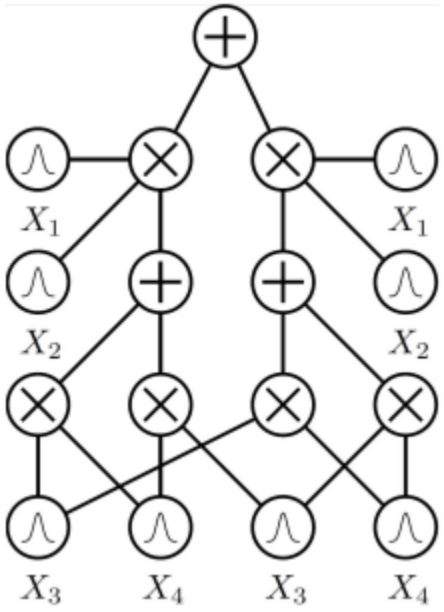
Stacked as a circuit



Probabilistic Circuits

Hierarchical Mixtures of Simple Factorized Distributions

Tractability for probabilistic inference is achieved via structural properties



Inference Queries

Probabilistic Circuits

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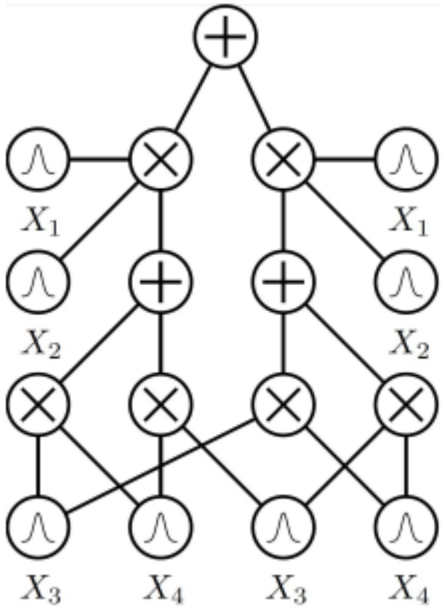

Inference Queries

Evidential Inference: $p(X_1, X_2, X_3, X_4)$

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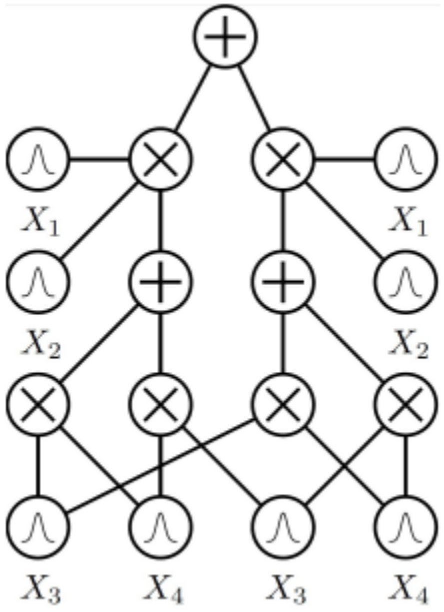

Inference Queries

Evidential Inference:	$p(X_1, X_2, X_3, X_4)$
Marginal Inference:	$p(X_1)$

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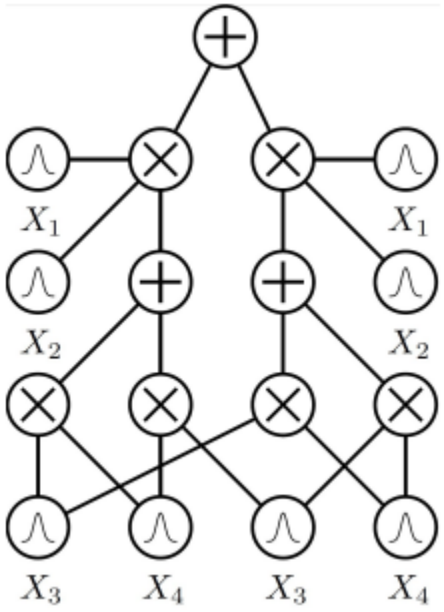

Inference Queries

Evidential Inference:	$p(X_1, X_2, X_3, X_4)$
Marginal Inference:	$p(X_1)$
Conditional Inference:	$p(X_1 \mid X_2, X_3, X_4)$

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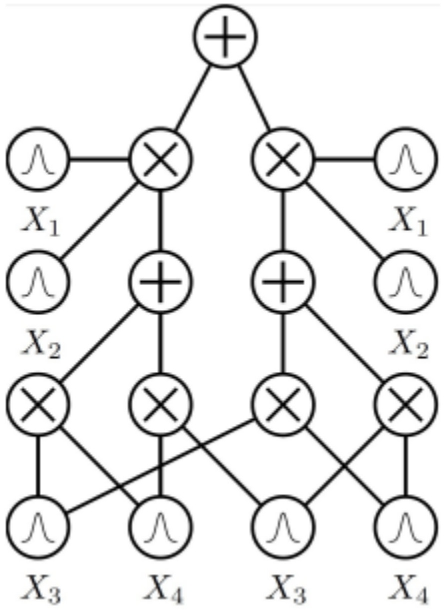

Inference Queries

Evidential Inference:	$p(X_1, X_2, X_3, X_4)$
Marginal Inference:	$p(X_1)$
Conditional Inference:	$p(X_1 \| X_2, X_3, X_4)$
MAP Inference:	$\text{argmax}_{X_1}\ p(X_1 \| X_2, X_3, X_4)$

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Structural Properties

Smoothness	Children of sum nodes have same scope

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Determinism	Children of sum nodes have disjoint support
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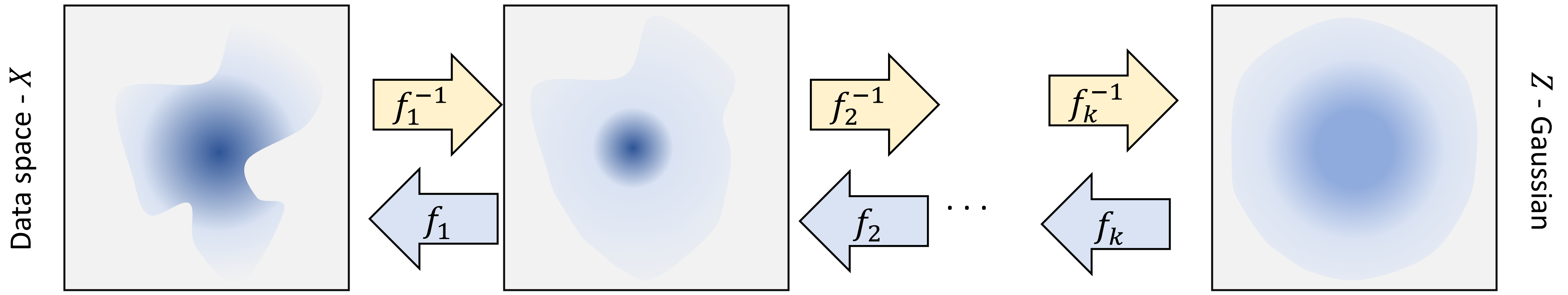
Normalizing Flows

Model data distributions using Invertible transformations and the change of variables formula



Normalizing Flows

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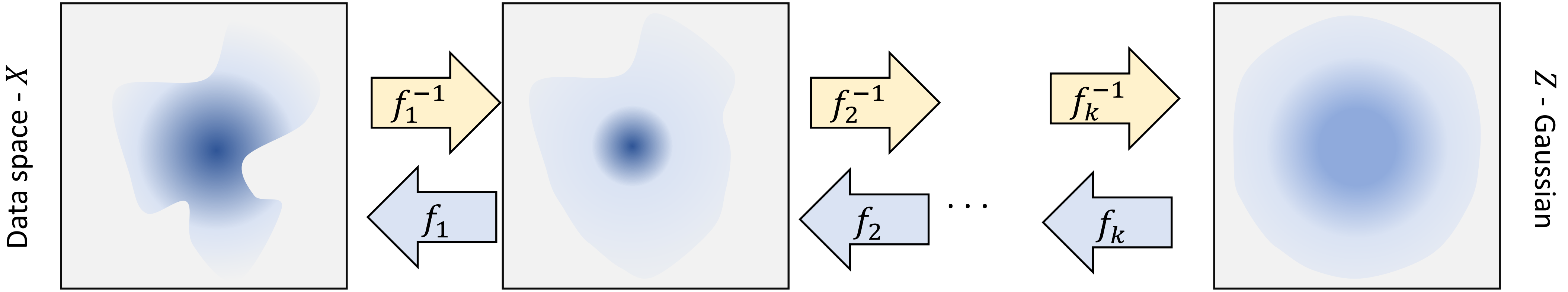
Change of Variables: Z and X be random variables which are related by a mapping $f : \mathbb{R}^n \to \mathbb{R}^n$ such that $X = f(Z)$ and $Z = f^{-1}(X)$. Then

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



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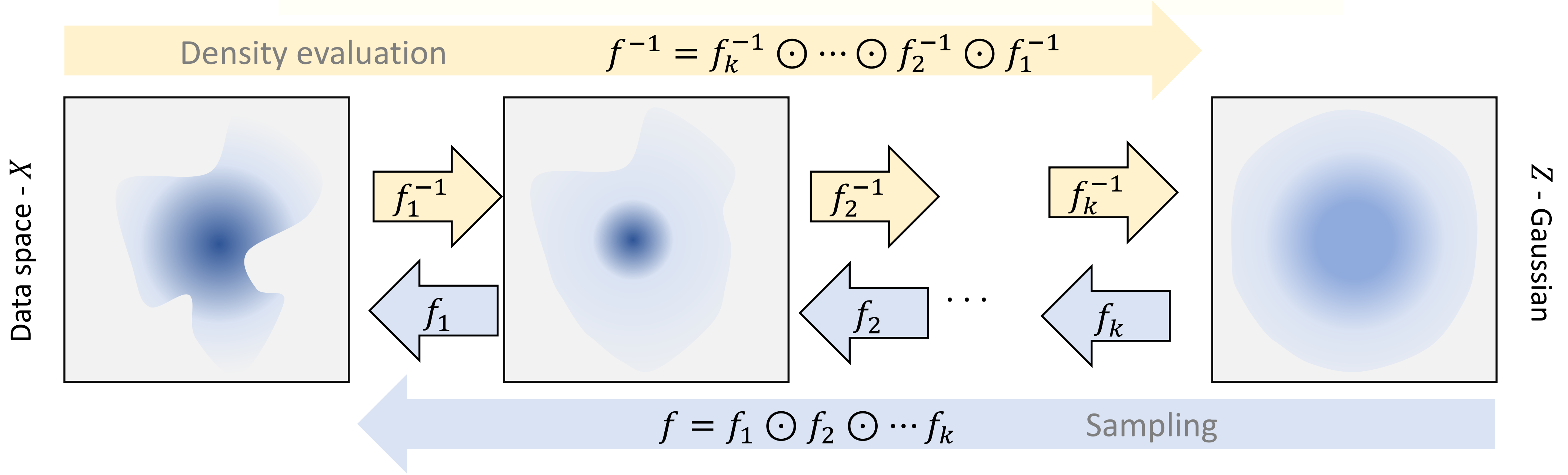

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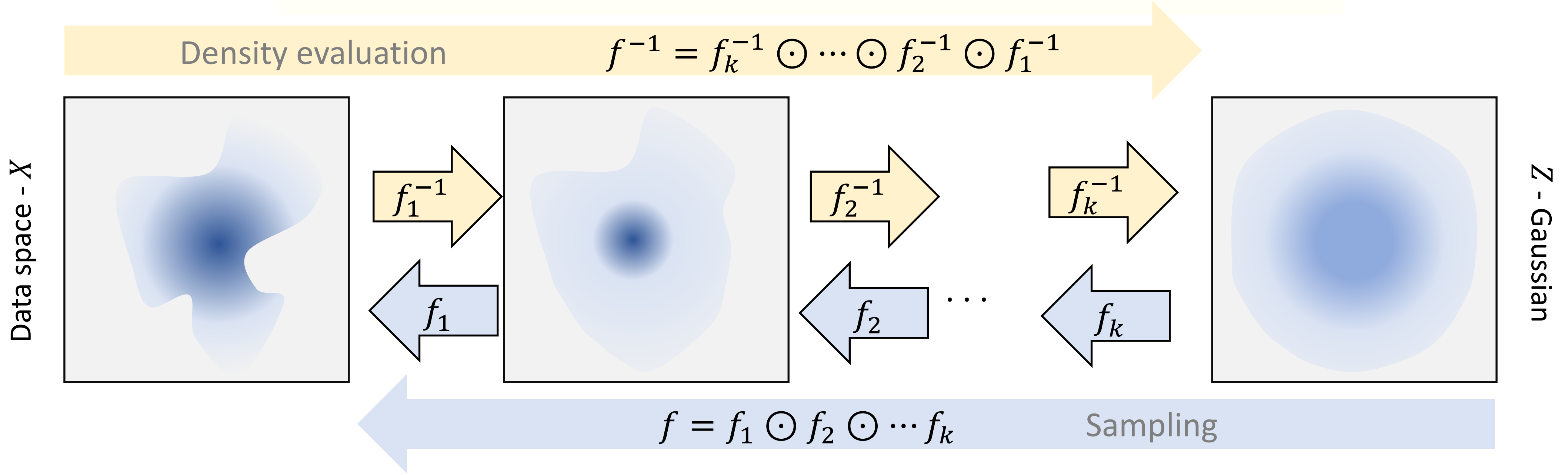


Parameterize efficient invertible transformations using **neural** networks

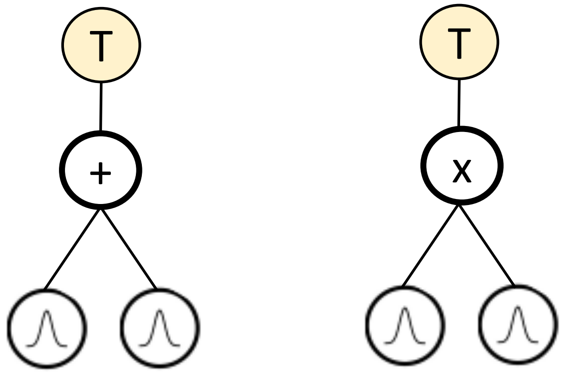
Supports **exact** density evaluation

More expressive than Probabilistic Circuits

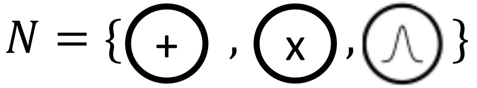
Integrating Flows with Probabilistic Circuits

Use the change of variables within PCs

Introduce new **transform nodes** in PCs



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



Transform nodes
Represents **normalizing** flows
Adds expressivity

Sum-Product Transform Network
(Pevny et. Al 2020)

Integrating Flows with Probabilistic Circuits

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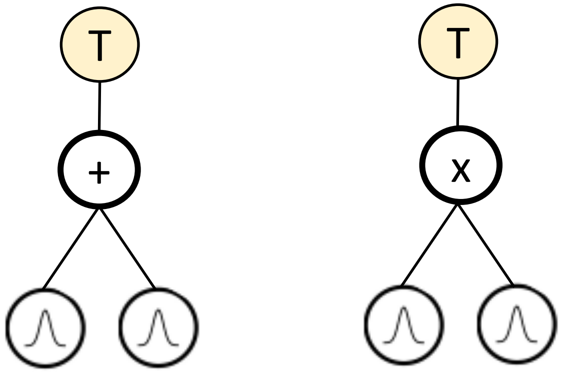

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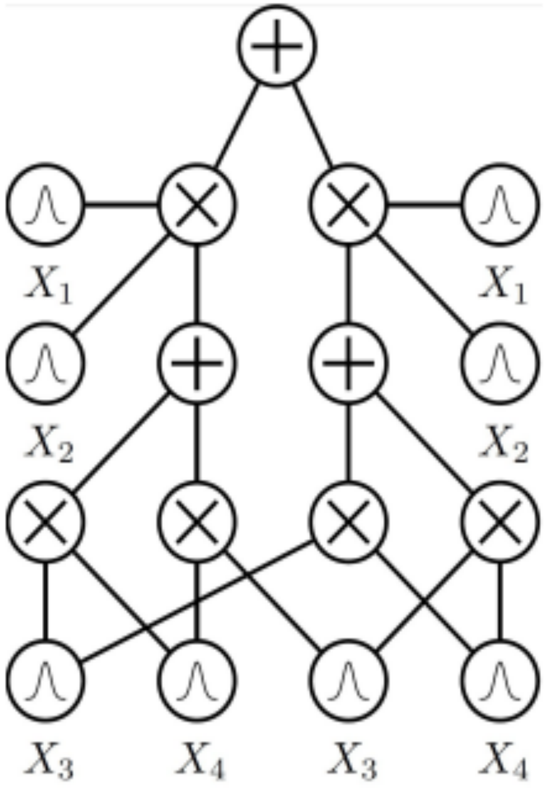
Probabilistic Circuit



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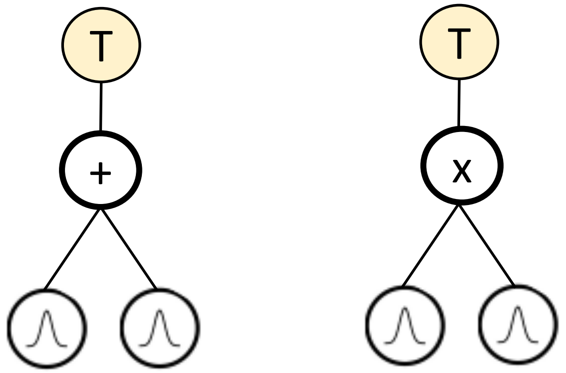

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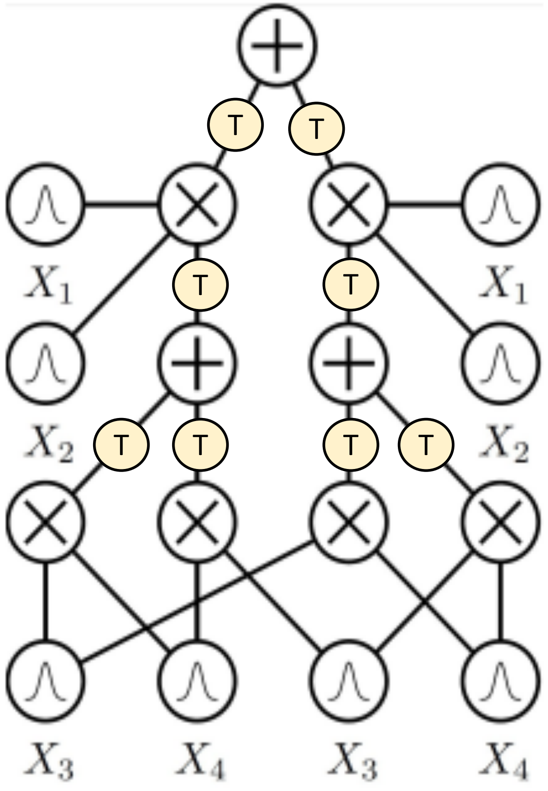

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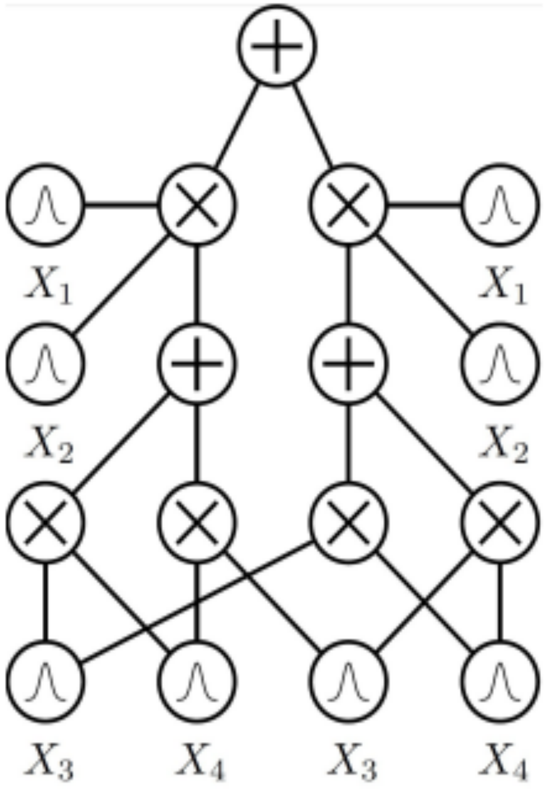

Place transform nodes arbitrarily in a PC

Integrating Flows with Probabilistic Circuits

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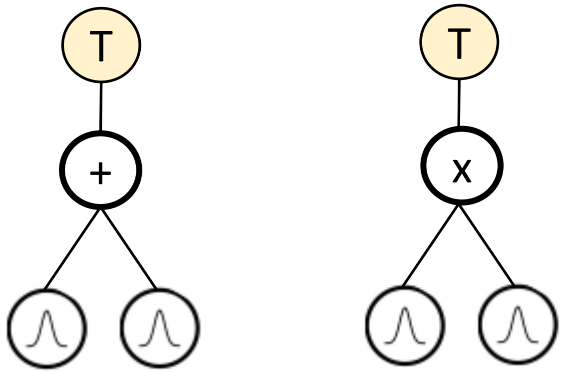

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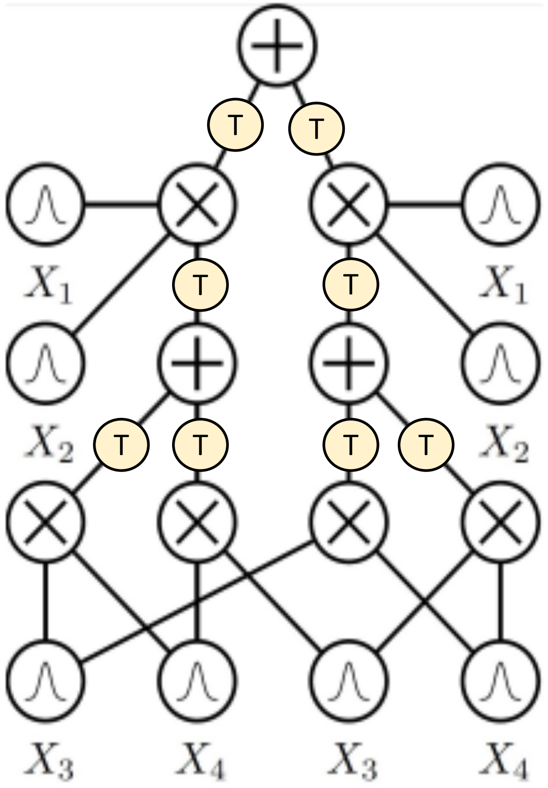

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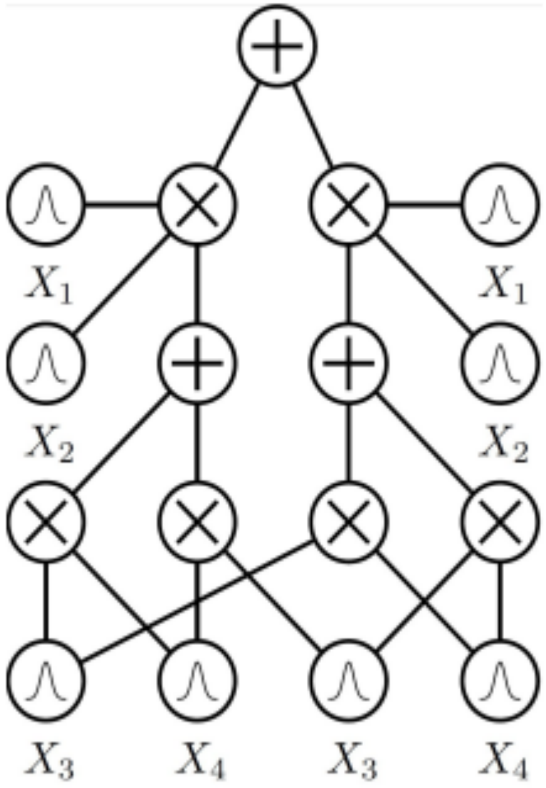

Place transform nodes arbitrarily in a PC

Use invertible **affine** transformations

Integrating Flows with Probabilistic Circuits – Our Work

Understanding the Pathologies of Sum-Product Transform Networks

Placing **transform nodes** arbitrarily in a PC can **violate** its **decomposability** property
Inference becomes **Intractable** for Marginal, Conditional, and MAP

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Probabilistic Circuits Smoothness and Decomposability allowed **pushing down** integrals to enable tractability

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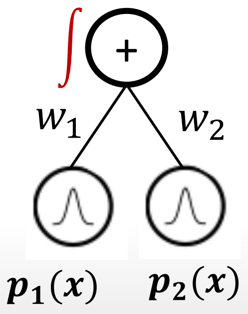
$$\int p(\boldsymbol{x})\, d\boldsymbol{x} = \int w_1\, p_1(\boldsymbol{x}) + w_2 p_2(\boldsymbol{x})\, d\boldsymbol{x}$$



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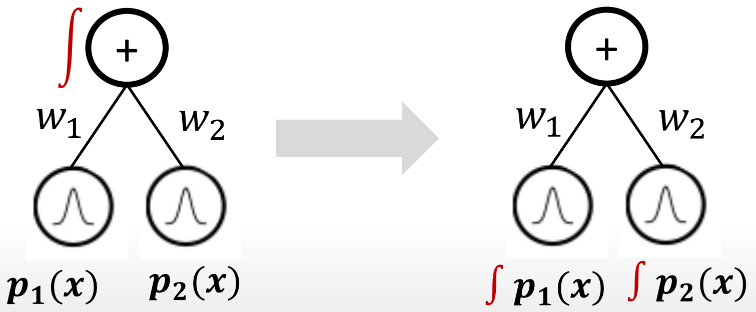

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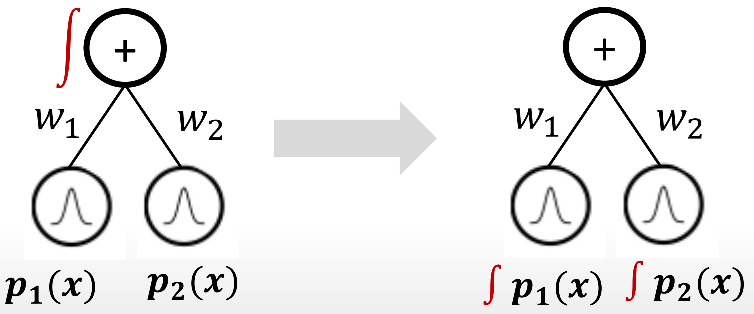

Decomposable Product Node

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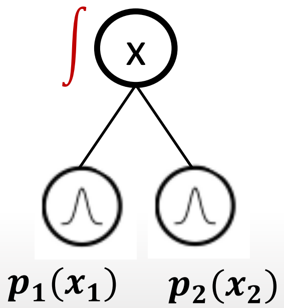

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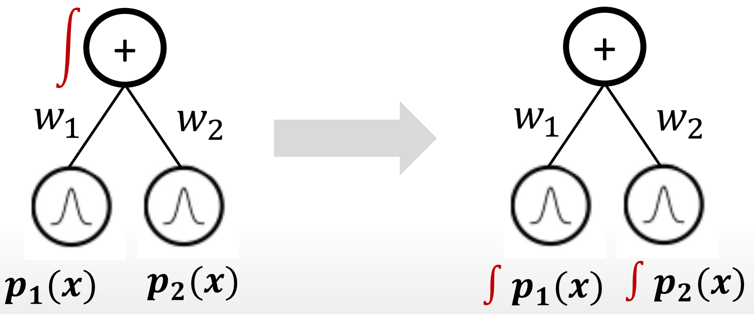

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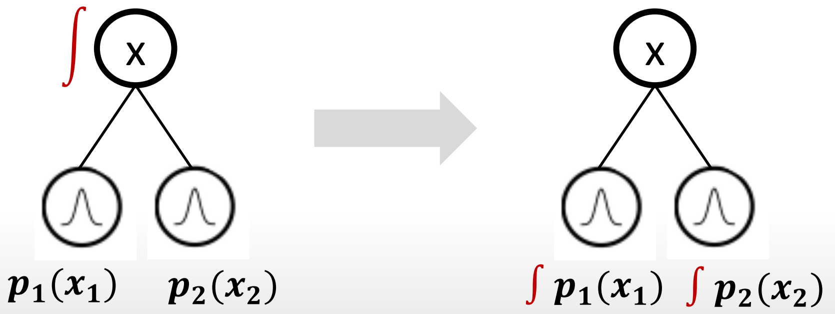

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Sum Product Transform Networks	Can you still push down integrals over transform nodes ?

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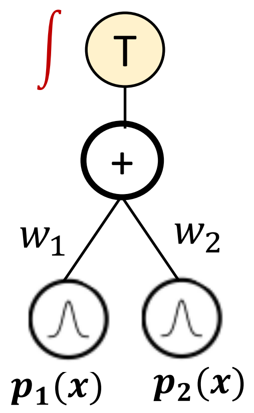
Sum Product Transform Networks Can you still push down integrals over transform nodes ?

Integrals on **Transform** Nodes **over Sum** Node

$$\int p(\boldsymbol{x})\, d\boldsymbol{x}$$

$$= \int T(+(\boldsymbol{x}))d\boldsymbol{x} = \int +(f(\boldsymbol{x}))|\det J_f|\ d\boldsymbol{x}$$

$$= \int [w_1 p_1(f(\boldsymbol{x})) + w_2 p_2(f(\boldsymbol{x}))]\, |\det J_f|\ d\boldsymbol{x}$$



Integrating Flows with Probabilistic Circuits – Our Work

Understanding the Pathologies of Sum-Product Transform Networks

Sum Product Transform Networks Can you still push down integrals over transform nodes ?

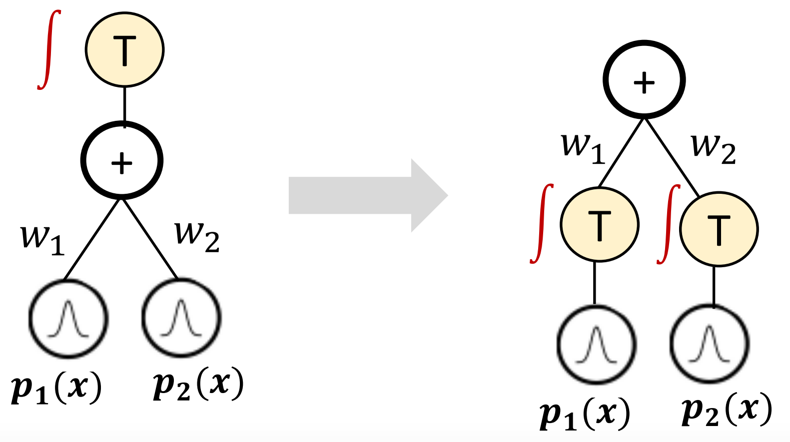
Integrals on **Transform** Nodes **over Sum** Node

$$\int p(\boldsymbol{x})\, d\boldsymbol{x}$$

$$= \int T(+(\boldsymbol{x}))d\boldsymbol{x} = \int +(f(\boldsymbol{x}))|\det J_f|\ d\boldsymbol{x}$$

$$= \int [w_1 p_1(f(\boldsymbol{x})) + w_2 p_2(f(\boldsymbol{x}))]\ |\det J_f|\ d\boldsymbol{x}$$

$$= w_1 \int p_1(f(\boldsymbol{x}))|\det J_f| d\boldsymbol{x}\ + w_2 \int p_2(f(\boldsymbol{x}))|\det J_f| d\boldsymbol{x}$$



Integrating Flows with Probabilistic Circuits – Our Work

Pathologies of Sum-Product Transform Networks

Integrals on Transform Nodes over Product Node

$$\int p(\boldsymbol{x_1},\boldsymbol{x_2})\, d\boldsymbol{x} \qquad (d\boldsymbol{x} = d\boldsymbol{x_1} d\boldsymbol{x_2})$$

$$= \int T(\times(\boldsymbol{x_1},\boldsymbol{x_2}))\, d\boldsymbol{x}$$

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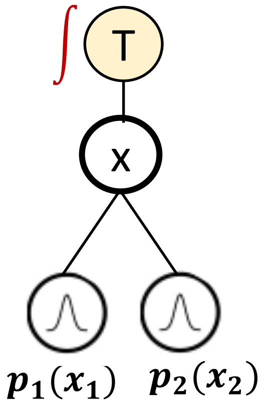

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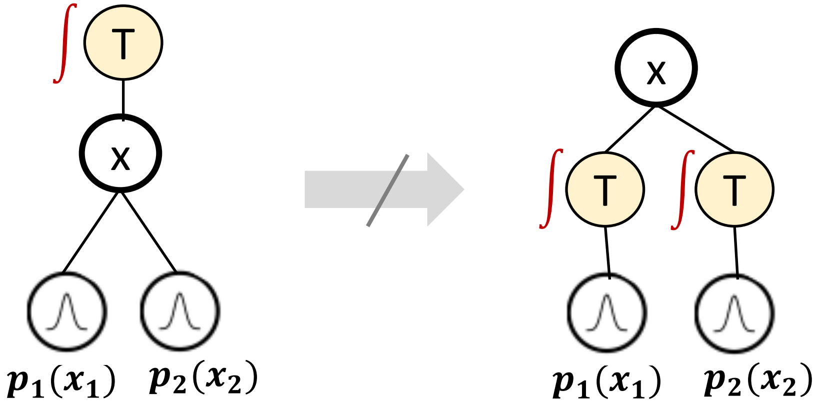

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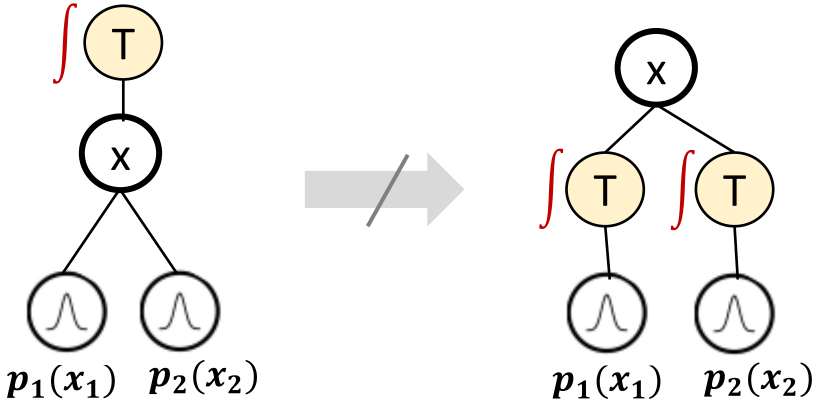

Transform nodes causes scopes of children of product nodes to overlap

Cannot push down integrals on transform nodes over products → Intractable for marginal, conditional and MAP

Integrating Flows with Probabilistic Circuits – Our Work

Defining Structural Properties for Transform Nodes

τ −Decomposability	When defined over a product node, f needs to transform the variables involved in the scope of its children **independently**

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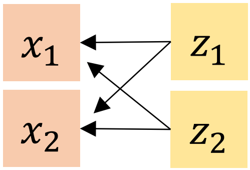
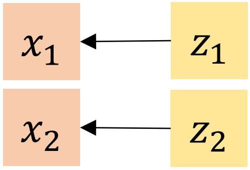


Not τ-Decomposable
$\boldsymbol{z} = f(\boldsymbol{x})$



τ-Decomposable
$\boldsymbol{z} = [z_1, z_2] = [f_1(x_1), f_2(x_2)]$

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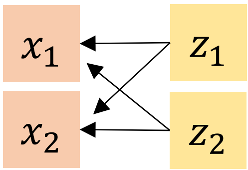

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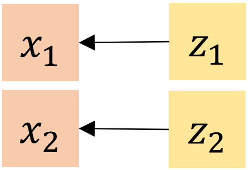

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Integrals on τ-Decomposable Transform Nodes over Product Node

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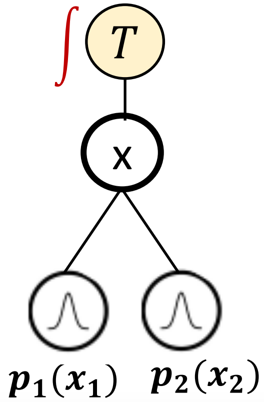

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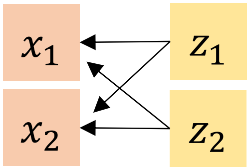

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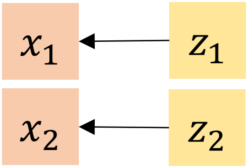

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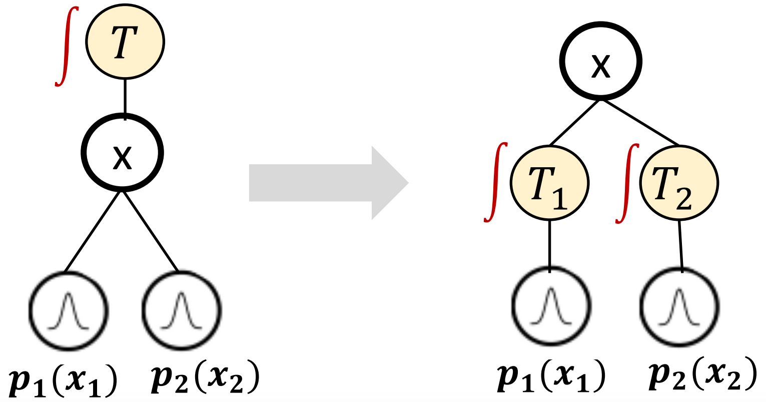

$$= \int p_1(f_1(\boldsymbol{x_1}))p_2(f_2(\boldsymbol{x_2}))|\det J_f| d\boldsymbol{x} = \left(\int p_1(f_1(\boldsymbol{x_1}))|\det J_{f_1}| d\boldsymbol{x_1}\right)\left(\int p_2(f_2(\boldsymbol{x_2}))|\det J_{f_2}| d\boldsymbol{x_2}\right)$$

Integrating Flows with Probabilistic Circuits – Our Work

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τ −Decomposability is a necessary condition for tractability

A sum-product-transform network is decomposable only if all of its transform nodes are τ −decomposable

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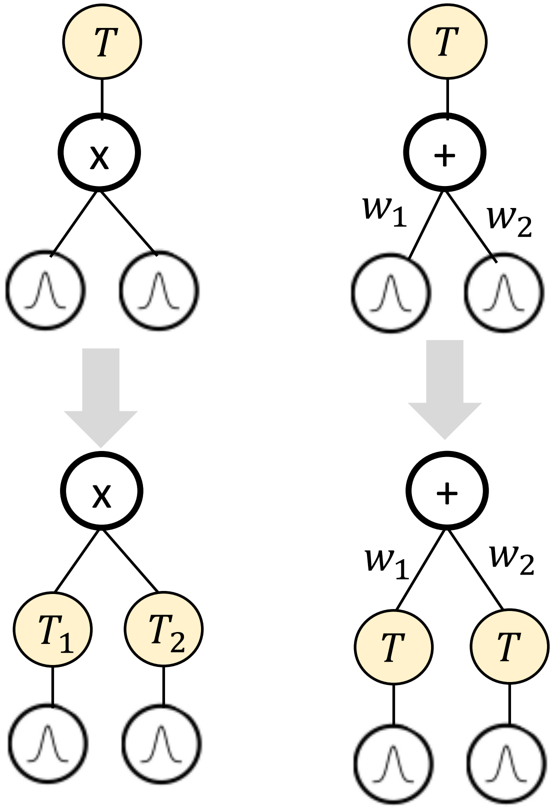
Implications of τ –decomposability



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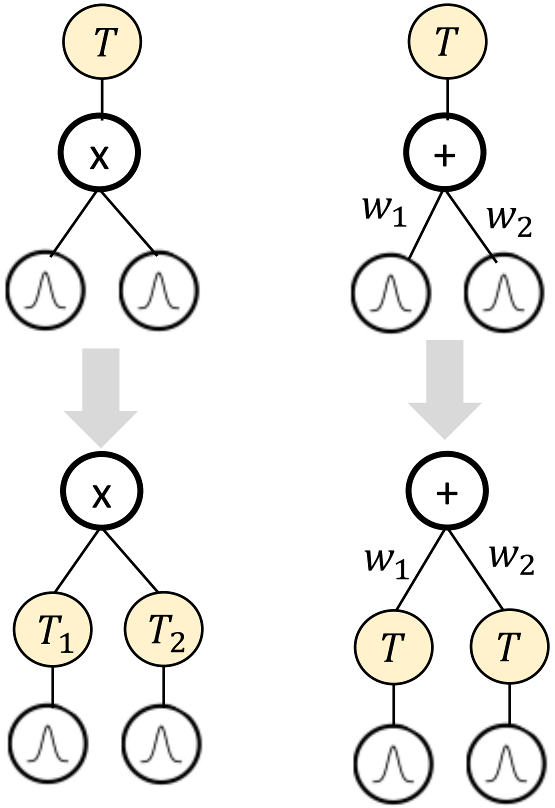

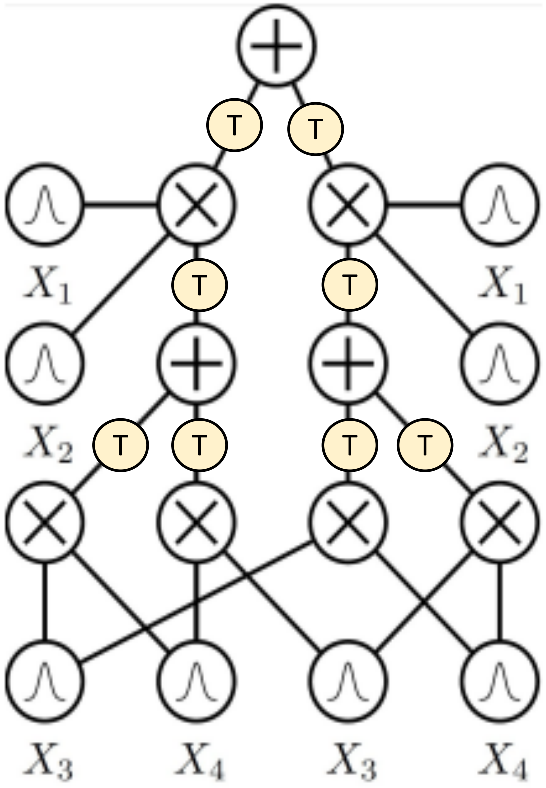

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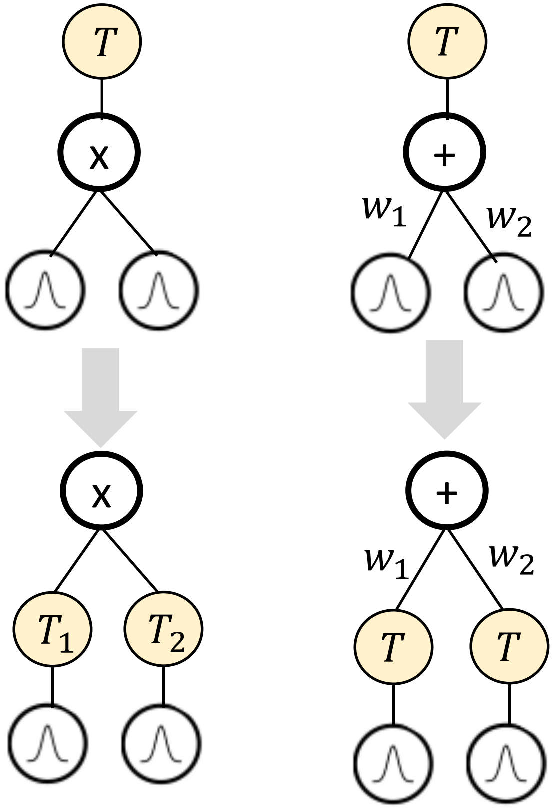

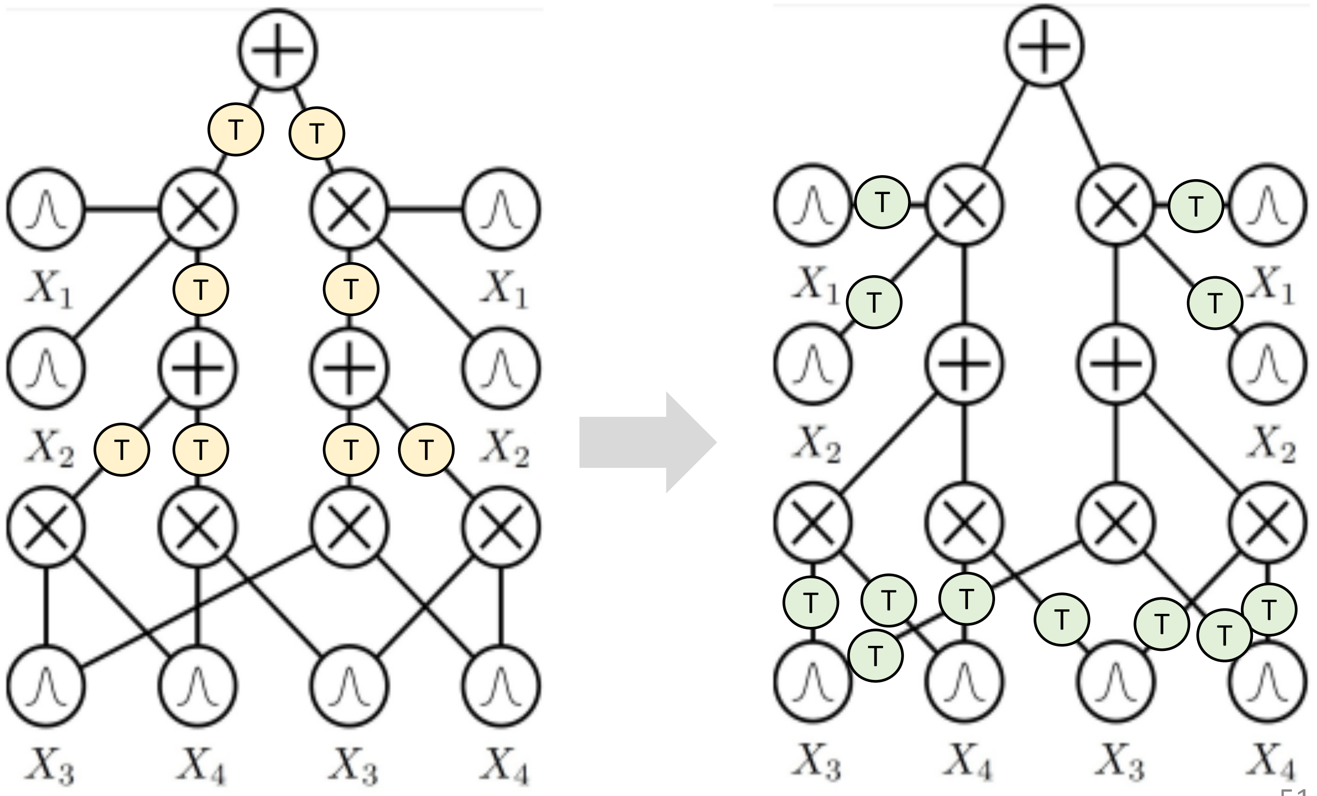

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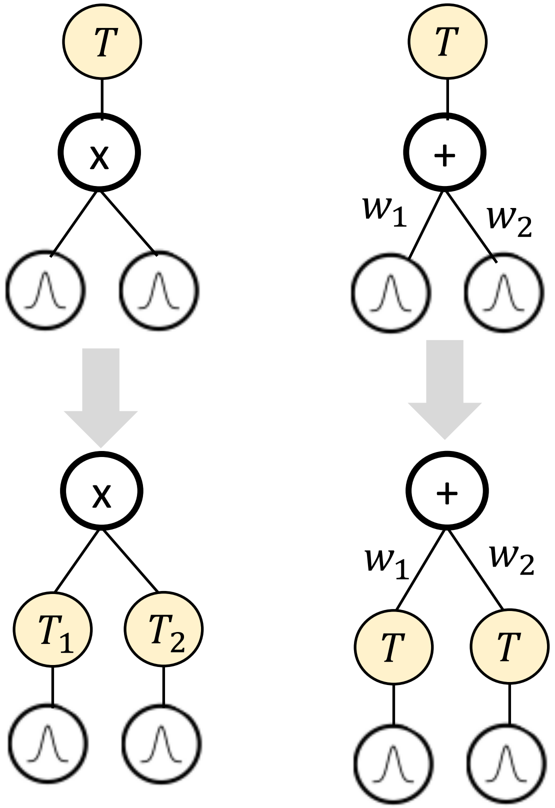
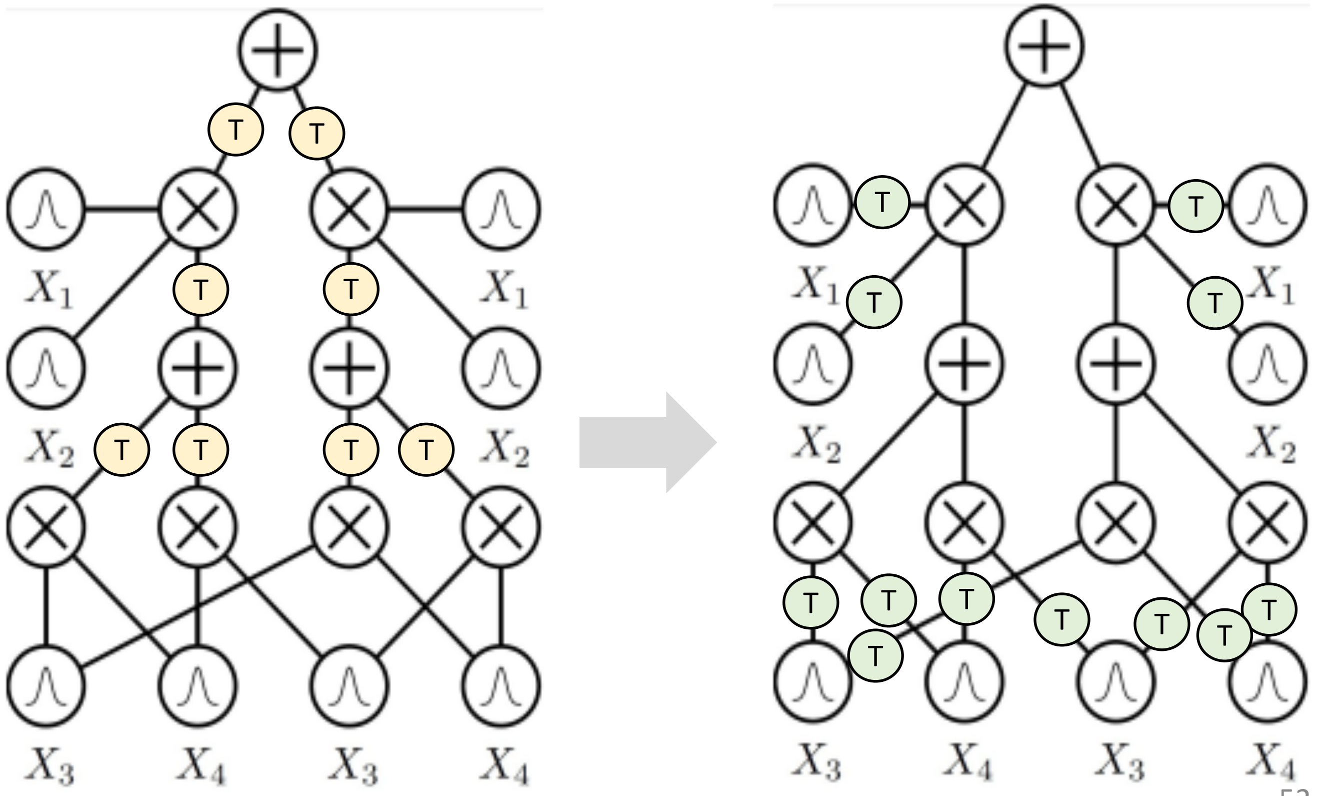
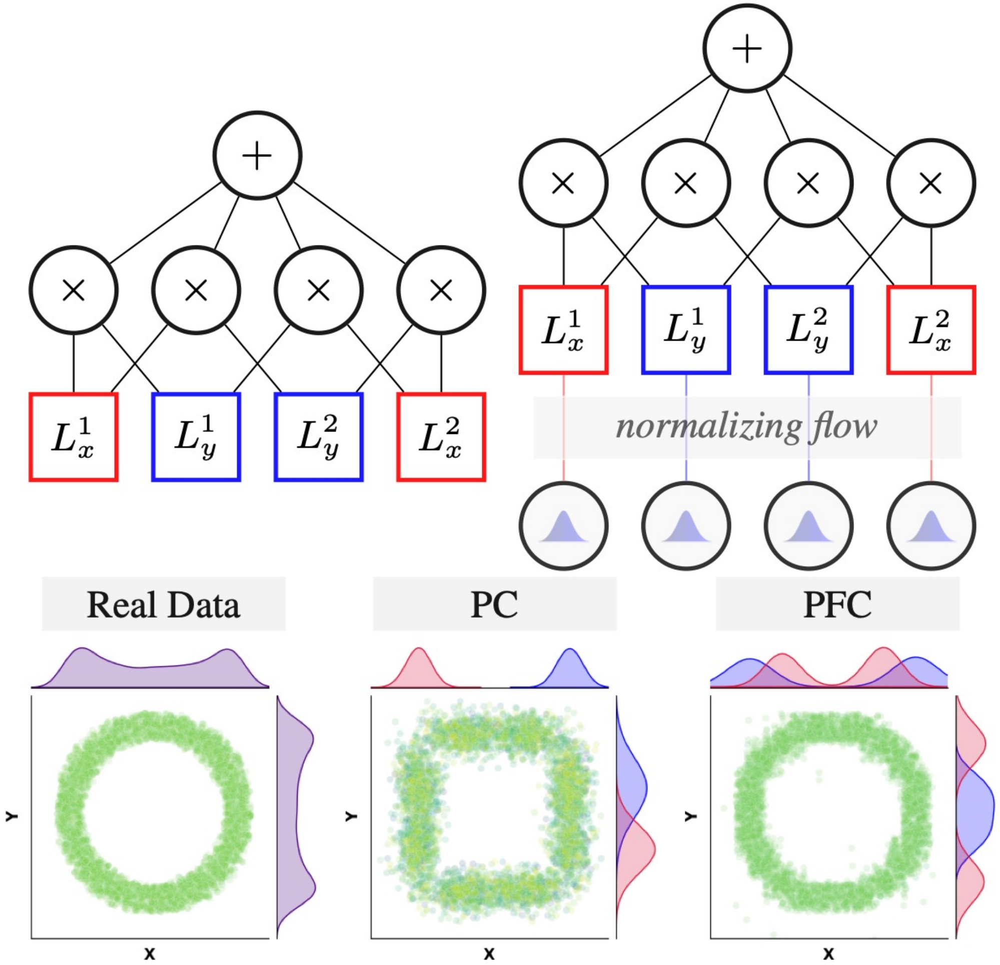
Implications of τ –decomposability

Reduces to having normalizing flows at the leaves!





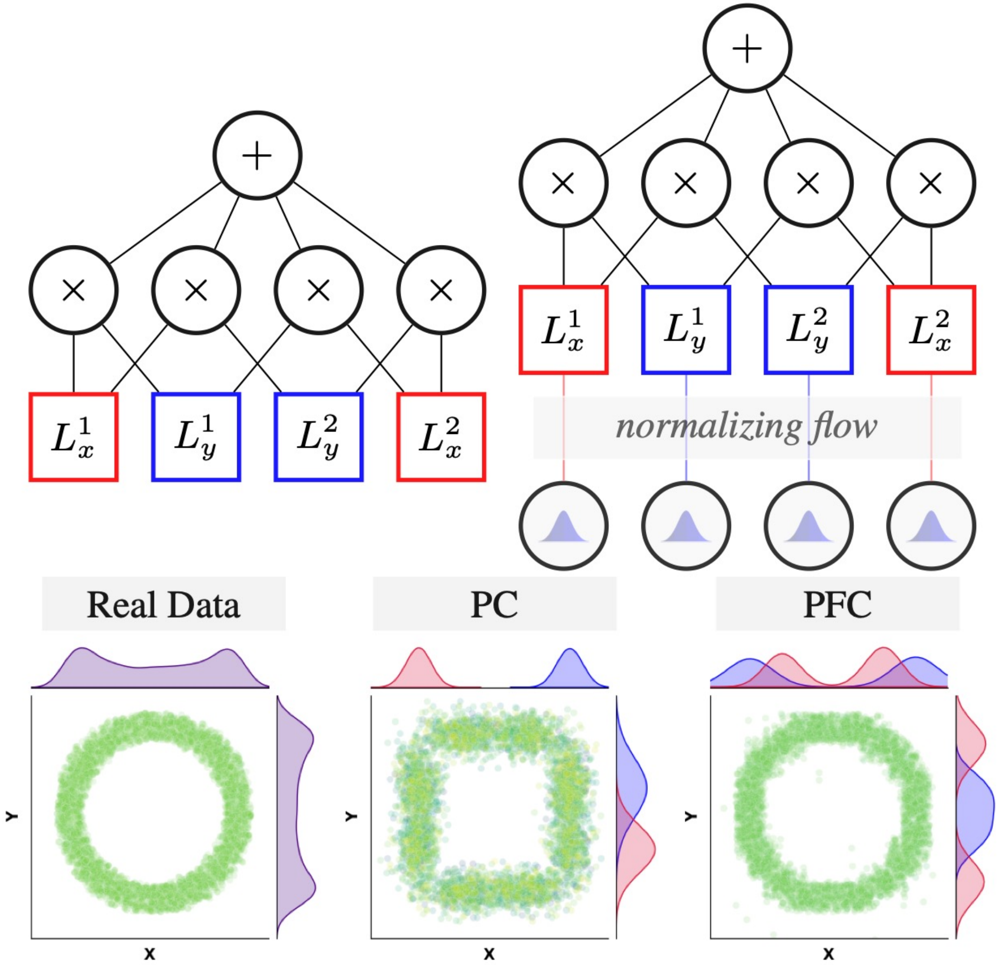
Probabilistic Flows Circuits



Has added Expressivity
Can model arbitrarily complex distributions at the leaves

Retains Tractability
As it encodes the same factorizations of the PC

Probabilistic Flows Circuits



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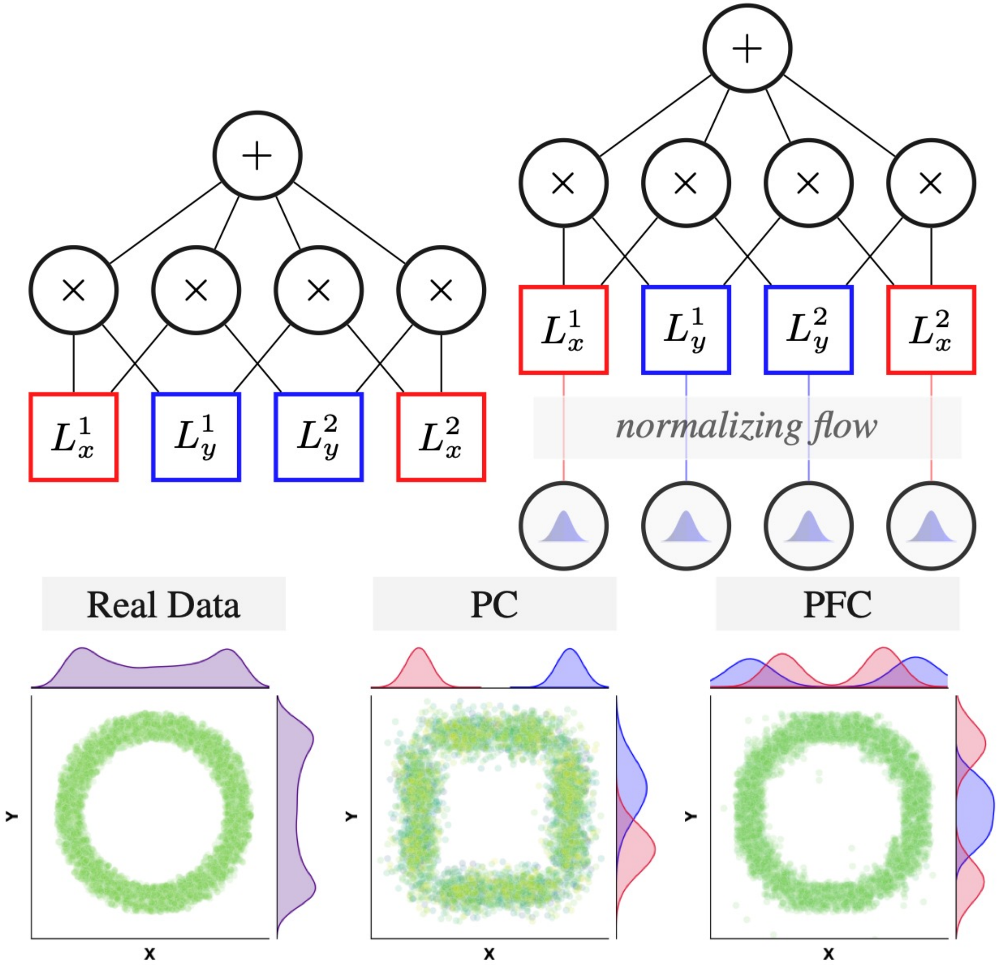

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Affine-transformed Gaussian leaf is still a Gaussian!

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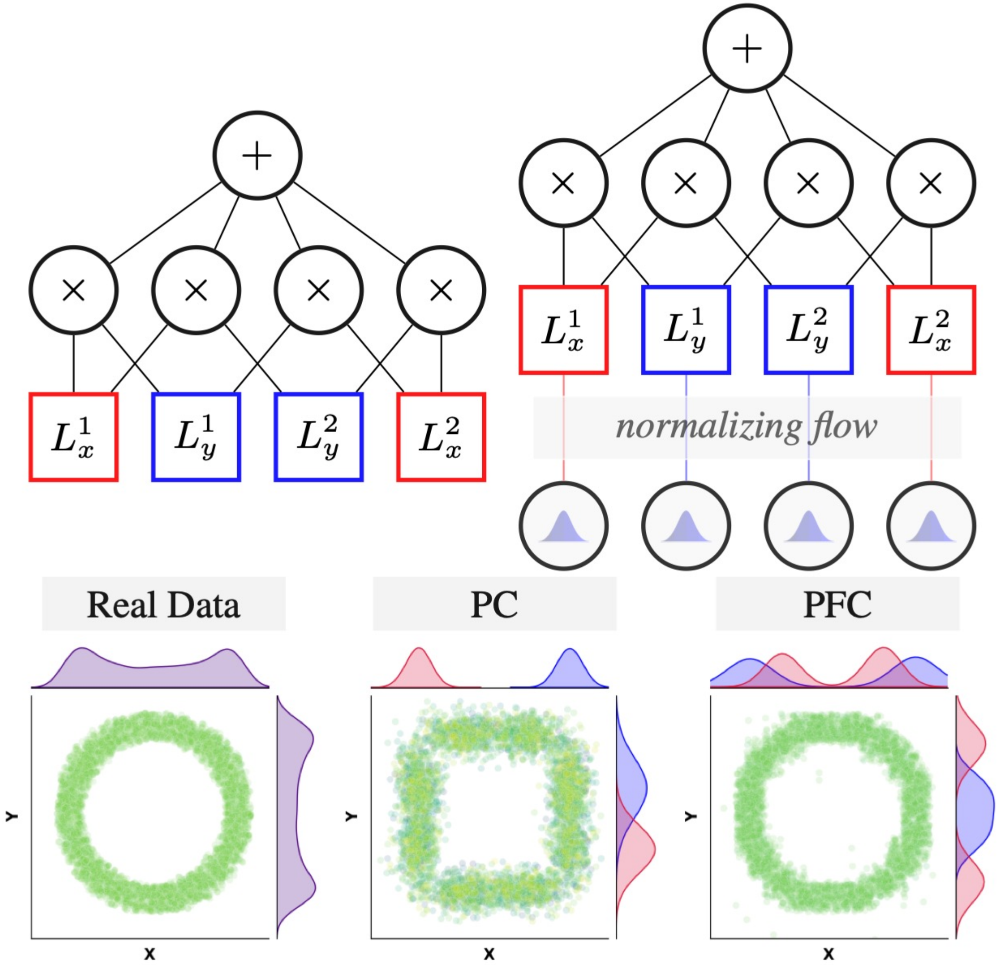

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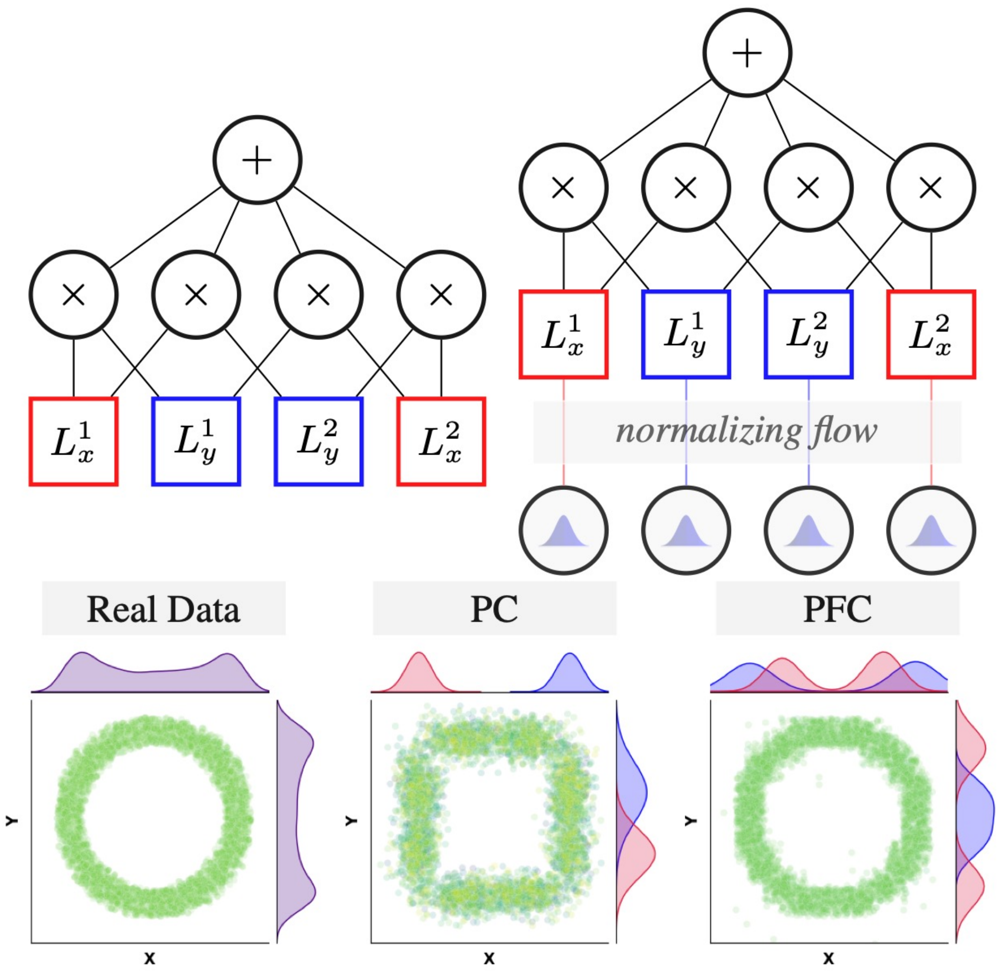

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MAP requires the ability to compute the **modes** of leaf distributions

PC
Unimodal Leaf
Easy to compute mode

PFC
Multimodal Leaf
Difficult to compute mode

Probabilistic Flows Circuits

Designing expressive transformations using linear rational splines

Spline-based flows are among SOTA

Splines - piecewise functions

Divide the data space into K bins and fit a polynomial function f_k within each

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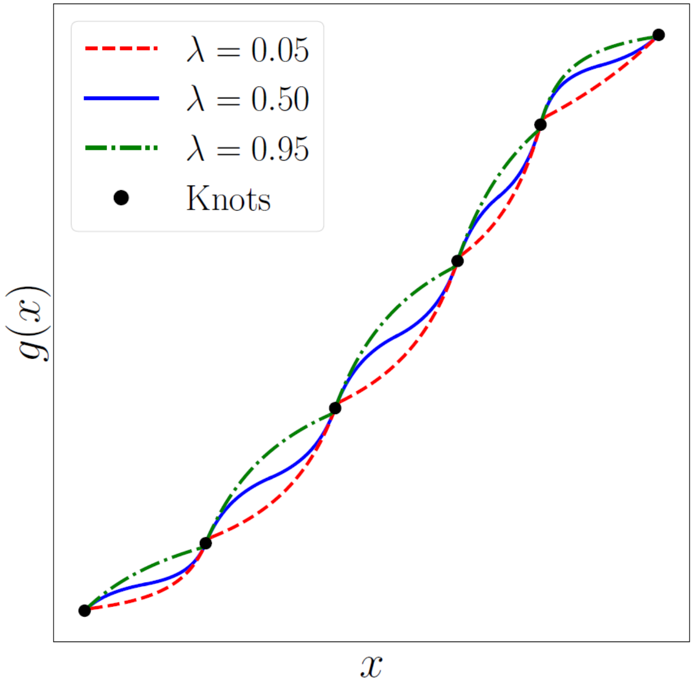
Linear Rational Splines (LRS)

Use monotone linear rational functions of the form $f(x) = \frac{ax+b}{cx+d}$



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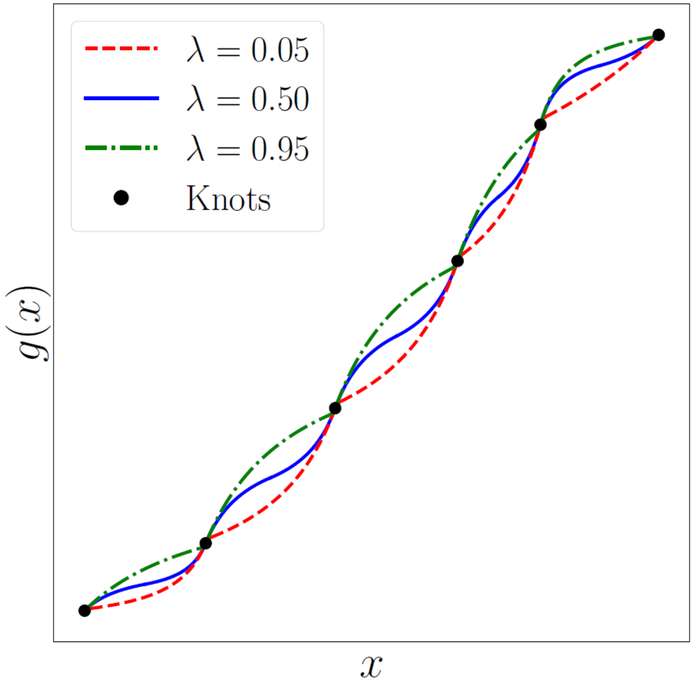

A PFC with LRS transformations is provably tractable for

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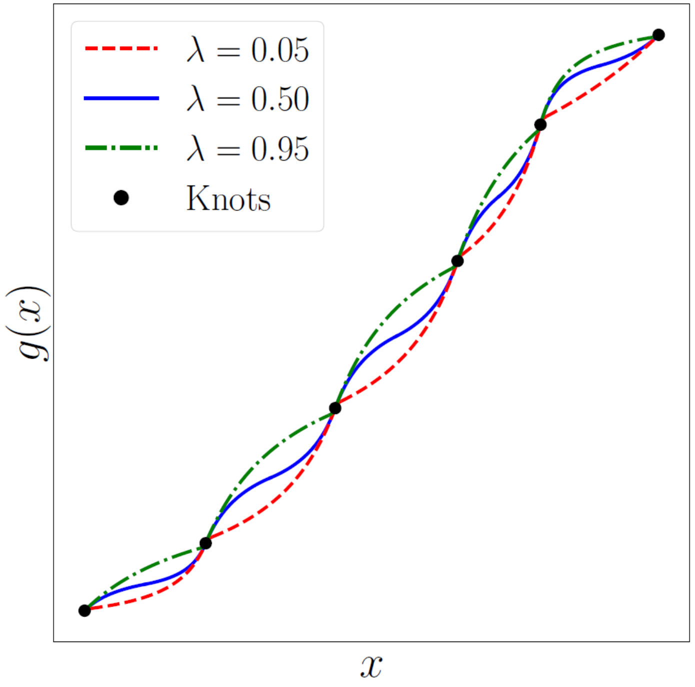

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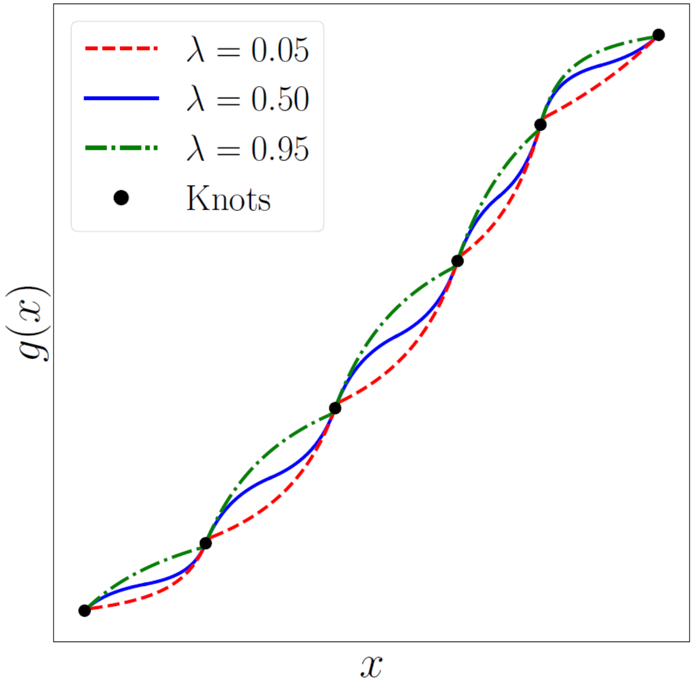

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  - smooth
- Marginal
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  - decomposable

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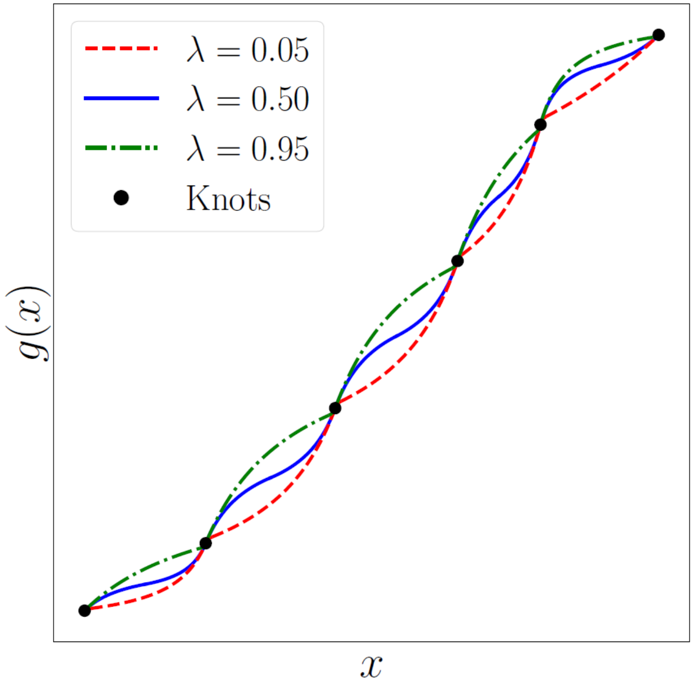

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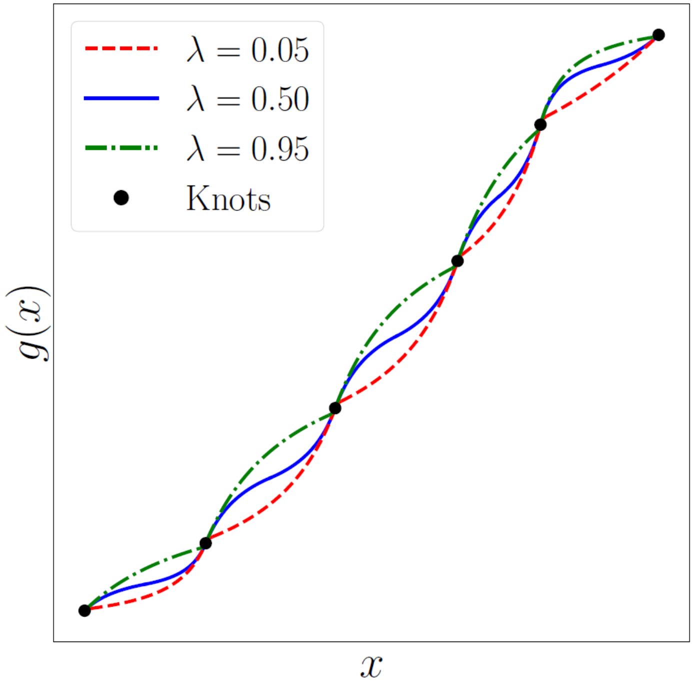

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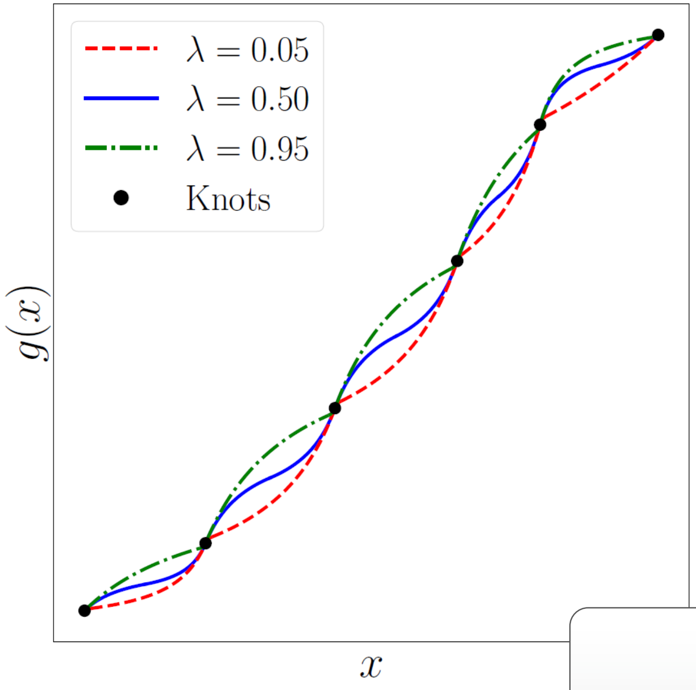

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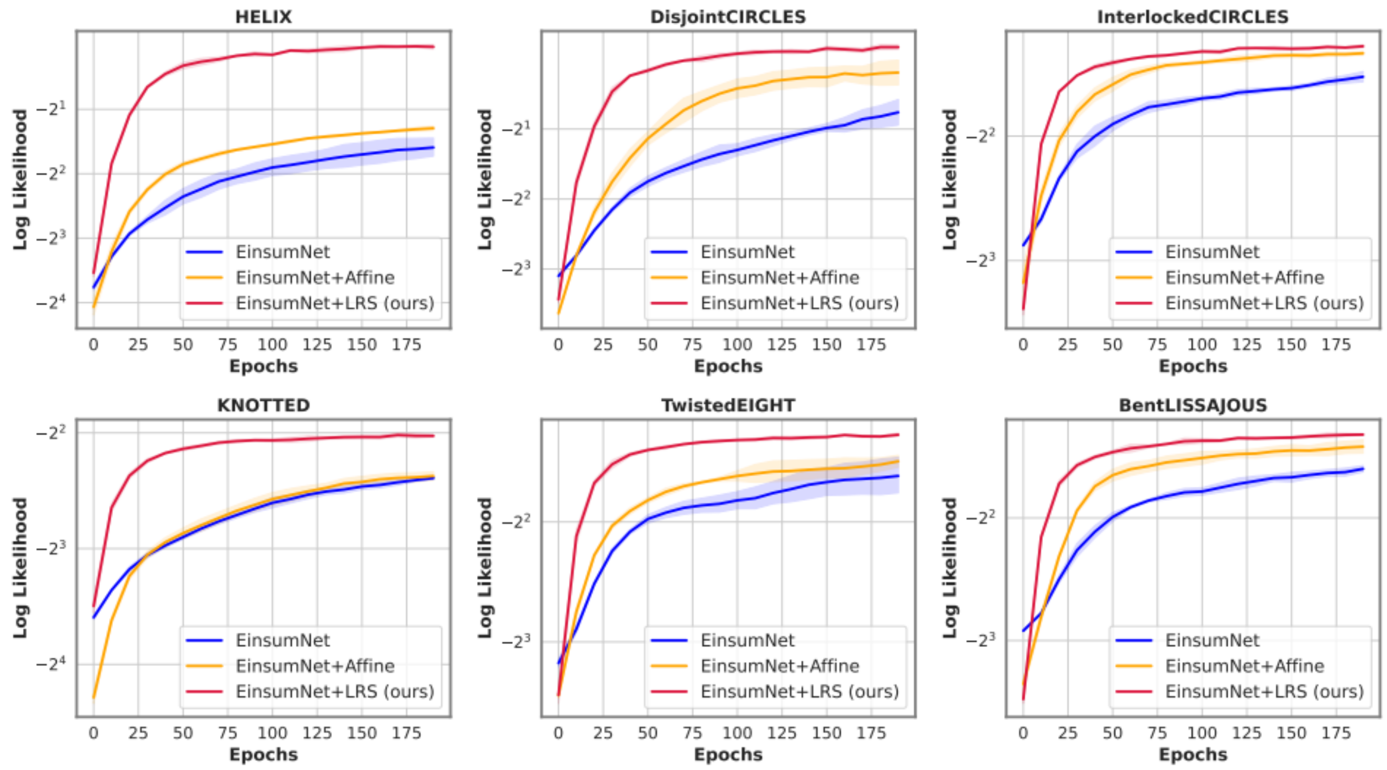
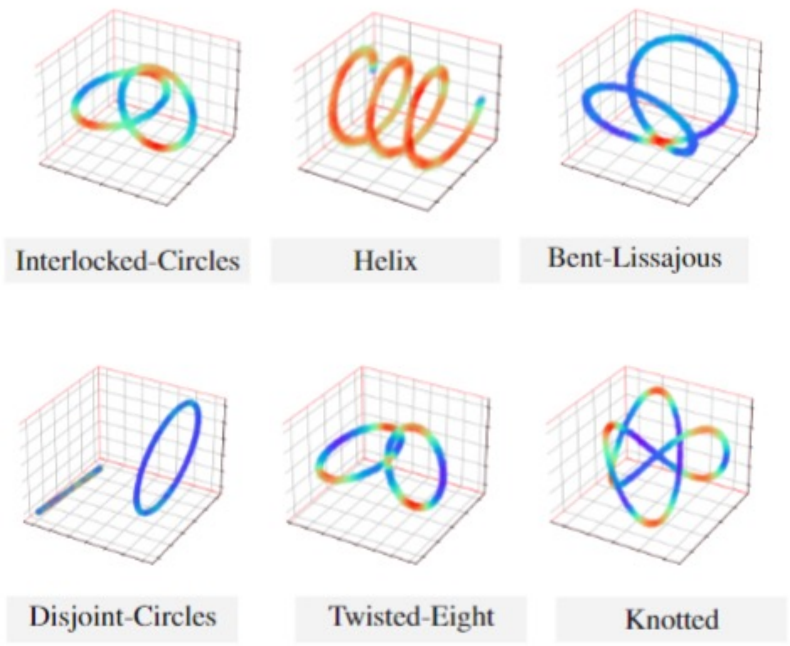
Other flow transformations that (provably) achieves the same ?

Probabilistic Flows Circuits

Experimental Results

Has added expressivity and learning efficiency over a PC - Better models the data





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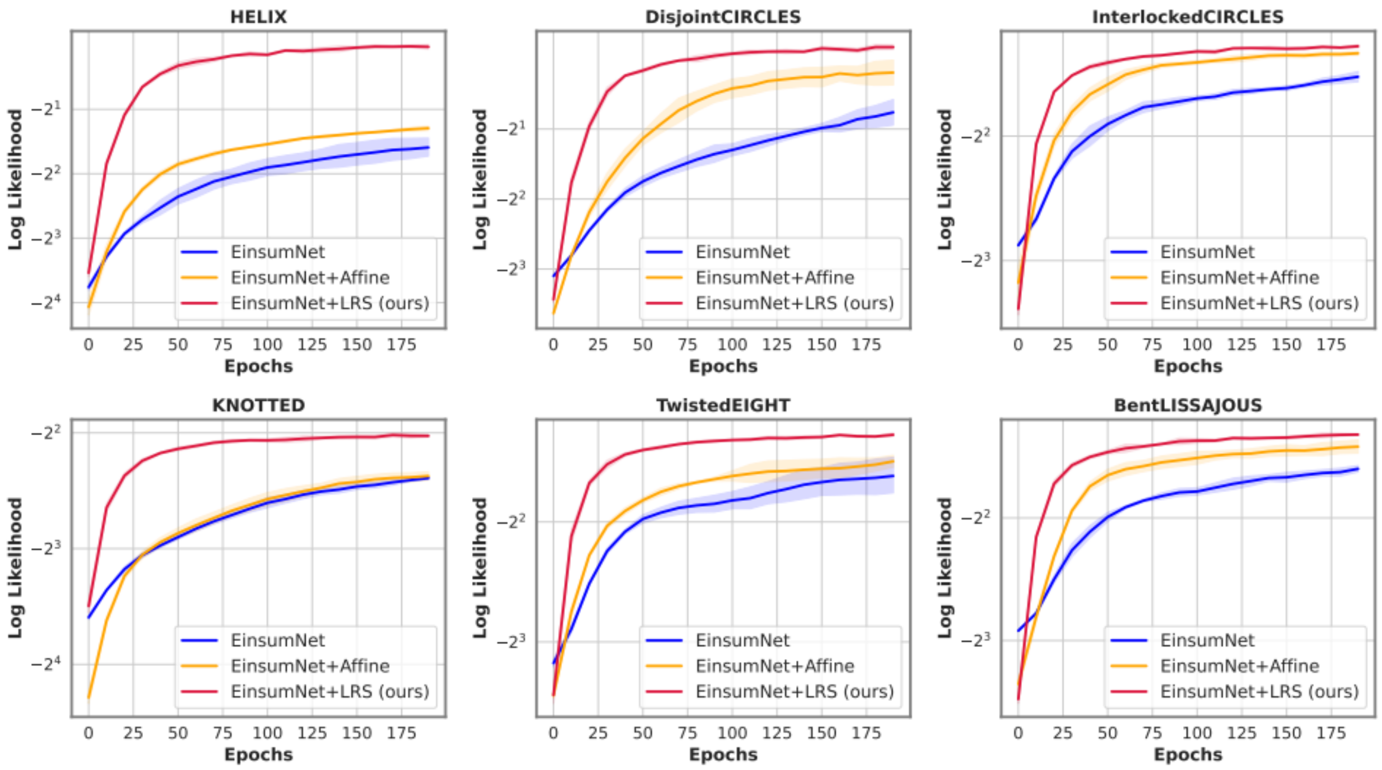
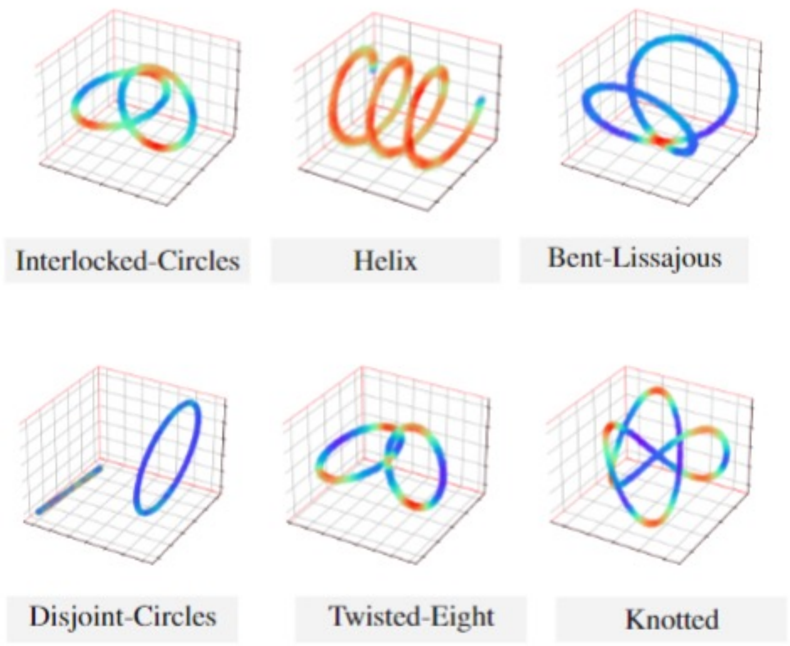




	POWER	GAS	MINIBOONE	HEPMASS	MNIST	Fashion-MNIST
MADE	-3.08 ± 0.03	3.56 ± 0.04	-15.59 ± 0.50	-20.98 ± 0.02	-1380.8 ± 4.8	-
Real NVP	-0.02 ± 0.01	4.78 ± 1.80	-13.55 ± 0.49	-19.62 ± 0.02	-1323.2 ± 6.6	-
MAF	0.14 ± 0.01	9.07 ± 0.02	-11.75 ± 0.44	-17.70 ± 0.02	-1300.5 ± 1.7	-
EinsumNet	0.20 ± 0.01	3.57 ± 0.08	-35.93 ± 0.06	-22.79 ± 0.05	-1015.1 ± 0.9	649.1 ± 0.3
Einsum+LRS	0.36 ± 0.01	4.79 ± 0.04	-34.21 ± 0.01	-22.46 ± 0.01	-959.4 ± 1.4	655.6 ± 0.6

Probabilistic Flows Circuits

Experimental Results

Retains Tractability – which can be exploited for downstream tasks

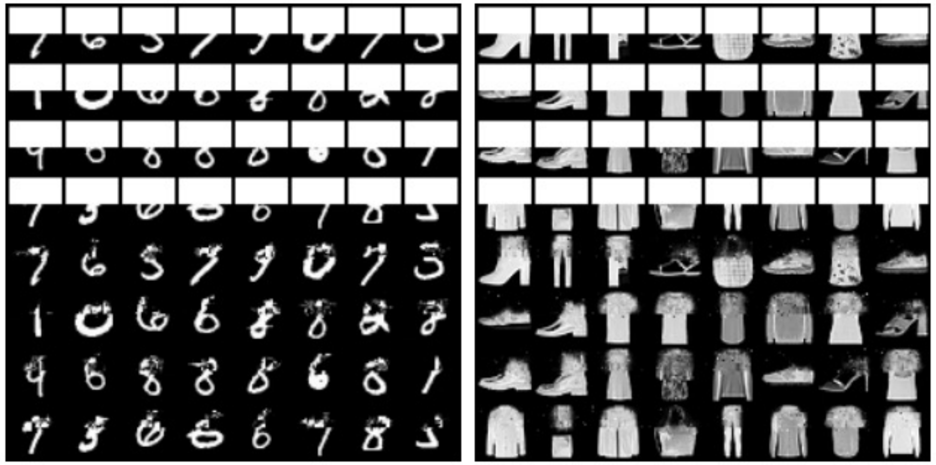
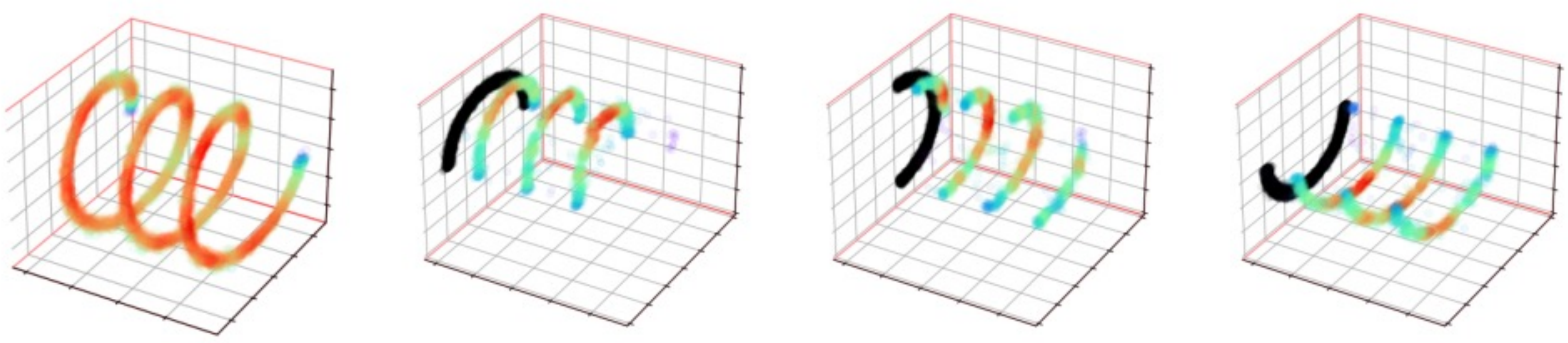


Image Inpainting

Can fill in missing data by sampling from conditional distributions



Can perform **controlled generation**

References

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Thank You! Questions?

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