

Semi-Discrete Normalizing Flows through Differentiable Tessellation

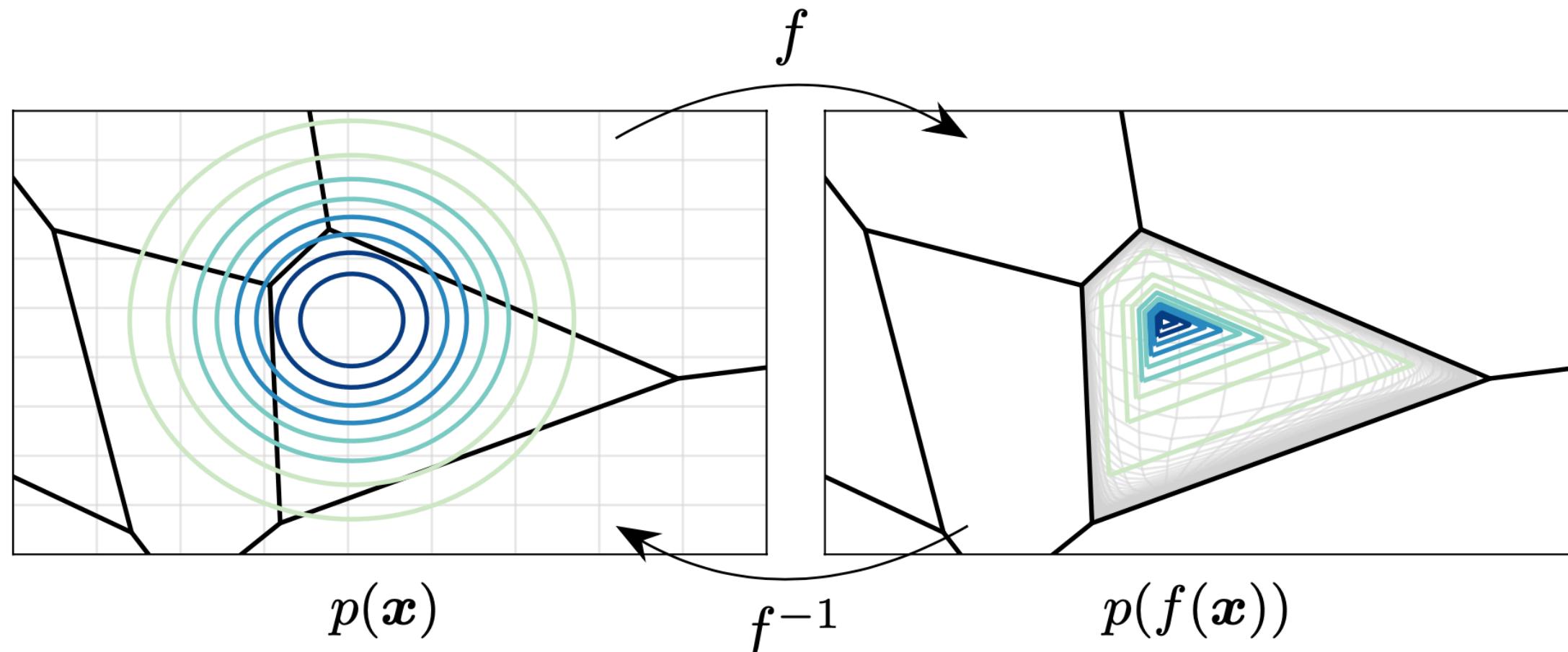
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Main Takeaways

- Differentiable tessellation + bijective mapping to construct normalizing flows on bounded supports.
- Maps between discrete & continuous distributions.
- Generalizes existing dequantization methods.
- Disjoint mixture models with $O(1)$ compute cost.

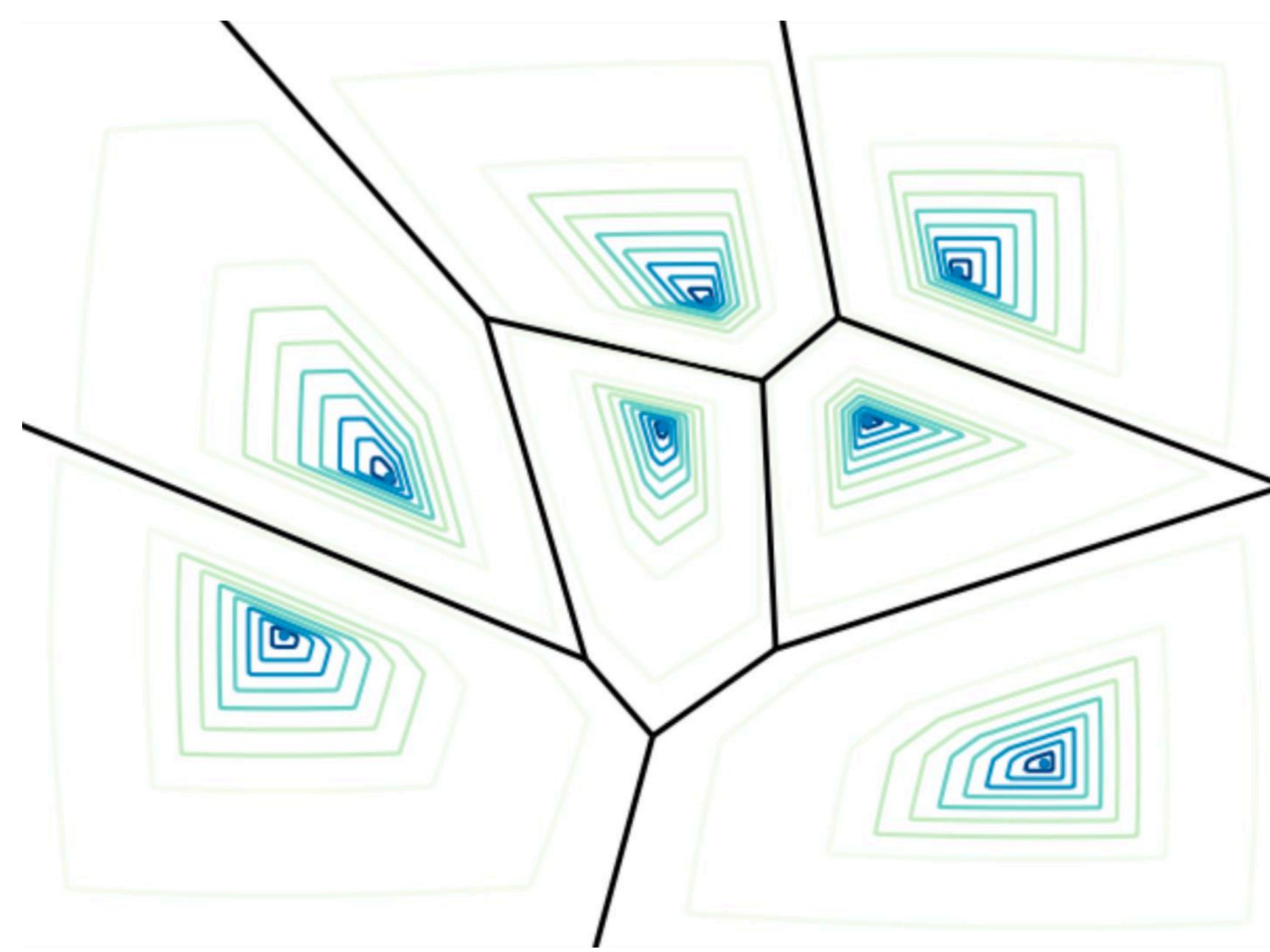
What?

Distributions with **bounded support**.



Why?

Combine lots of them with **disjoint support**.



Maps each continuous value to a discrete value.

$$\mathbb{1}_{[x \in A_y]}$$

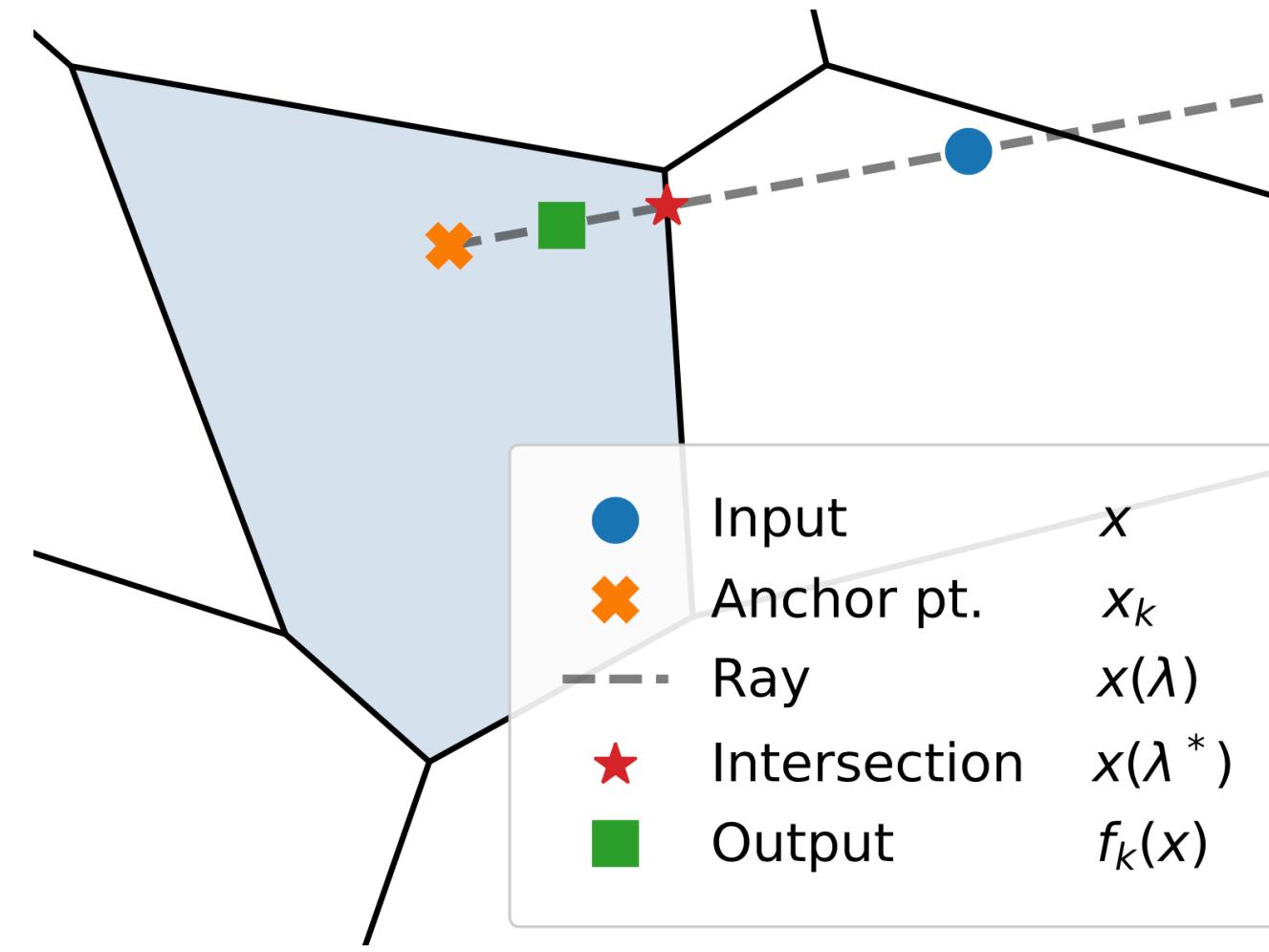
Maps each discrete value to a continuous distribution.

$$\log q(\mathbf{x}|\mathbf{y})$$

Bijective Mapping to Convex Supports

Parameterize Voronoi tessellation using anchor points.

Bijective map through 1D transformation:



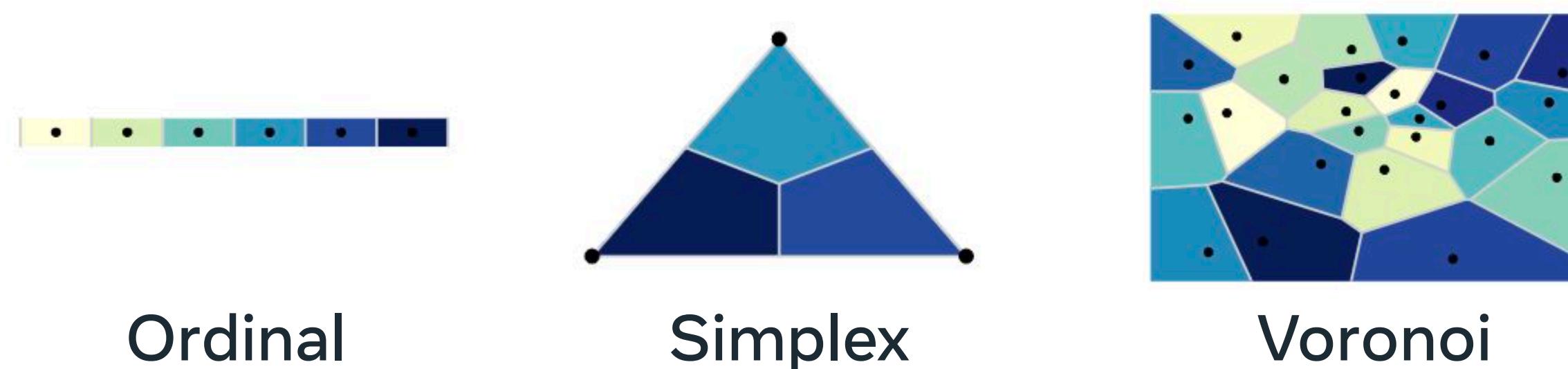
Log probability is easy to compute in closed form.

$$p_z(f(\mathbf{x})) = p_x(\mathbf{x}) \left| \det \frac{\partial f(\mathbf{x})}{\partial \mathbf{x}} \right|^{-1}$$

Voronoi Dequantization (Discrete Data)

Learns the map from discrete to continuous.

Does not couple dimension with #discrete values.



$$\begin{aligned} \log p(\mathbf{y}) &\geq \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x}|\mathbf{y})} [\log (\mathbb{1}_{[\mathbf{x} \in A_{\mathbf{y}}]} p(\mathbf{x})) - \log q(\mathbf{x}|\mathbf{y})] \\ &= \mathbb{E}_{\mathbf{x} \sim q(\mathbf{x}|\mathbf{y})} [\log p(\mathbf{x}) - \log q(\mathbf{x}|\mathbf{y})] \end{aligned}$$

Discrete model Density model (continuous) Dequantization model

Disjoint Mixture Modeling (Continuous Data)

Mixture models are expensive:

$$p(\mathbf{x}) = \sum_{k=1}^K p(\mathbf{x}|k)p(k)$$

Scales with number of components

But if components are disjoint:

$$\begin{aligned} p(\mathbf{x}) &= \sum_{k=1}^K \mathbb{1}_{[\mathbf{x} \in A_k]} p(\mathbf{x}|k)p(k) \\ &= p(\mathbf{x}|k=g(\mathbf{x}))p(k=g(\mathbf{x})) \end{aligned}$$

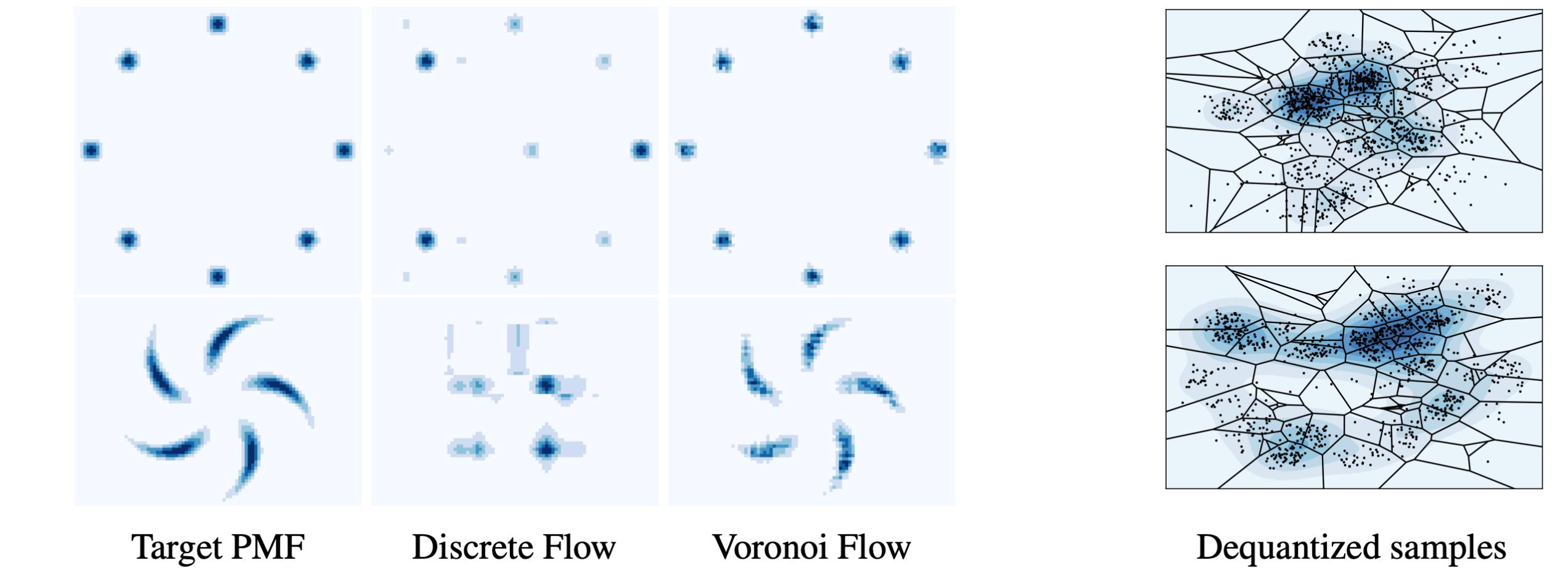
Disjoint subsets

Set identification function

Experiments

Can model complex relations between discrete data.

Learns to cluster discrete values with similar probabilities.



Beats existing dequantization approaches across many data modalities

Table 1: Discrete UCI data sets. Negative log-likelihood results on the test sets in nats.

Method	Connect4	Forests	Mushroom	Nursery	PokerHands	USCensus90
Voronoi Deq.	12.92 ± 0.07	14.20 ± 0.05	9.06 ± 0.05	9.27 ± 0.04	19.86 ± 0.04	24.19 ± 0.12
Simplex Deq.	13.46 ± 0.01	16.58 ± 0.01	9.26 ± 0.01	9.50 ± 0.00	19.90 ± 0.00	28.09 ± 0.08
BinaryArgmax Deq.	13.71 ± 0.04	16.73 ± 0.17	9.53 ± 0.01	9.49 ± 0.00	19.90 ± 0.01	27.23 ± 0.02
Discrete Flow	19.80 ± 0.01	21.91 ± 0.01	22.06 ± 0.01	9.53 ± 0.01	19.82 ± 0.03	55.62 ± 0.35

Table 2: Permutation-invariant discrete itemset modeling.

Model (Dequantization)	Retail (nats)	Accidents (nats)
CNF (Voronoi)	9.44 ± 2.34	7.81 ± 2.84
CNF (Simplex)	24.16 ± 0.21	19.19 ± 0.01
CNF (BinaryArgmax)	10.47 ± 0.42	6.72 ± 0.23
Determinantal Point Process	20.35 ± 0.05	15.78 ± 0.04

Table 3: Language modeling.

Dequantization	text8 (bpc)	enwik8 (bpc)
Voronoi ($D=2$)	1.39 ± 0.01	1.46 ± 0.01
Voronoi ($D=4$)	1.37 ± 0.00	1.41 ± 0.00
Voronoi ($D=6$)	1.37 ± 0.00	1.40 ± 0.00
Voronoi ($D=8$)	1.36 ± 0.00	1.39 ± 0.01
BinaryArgmax [18]	1.38	1.42
Ordinal [18]	1.43	1.44

Disjoint mixture modeling increases flexibility at no cost.

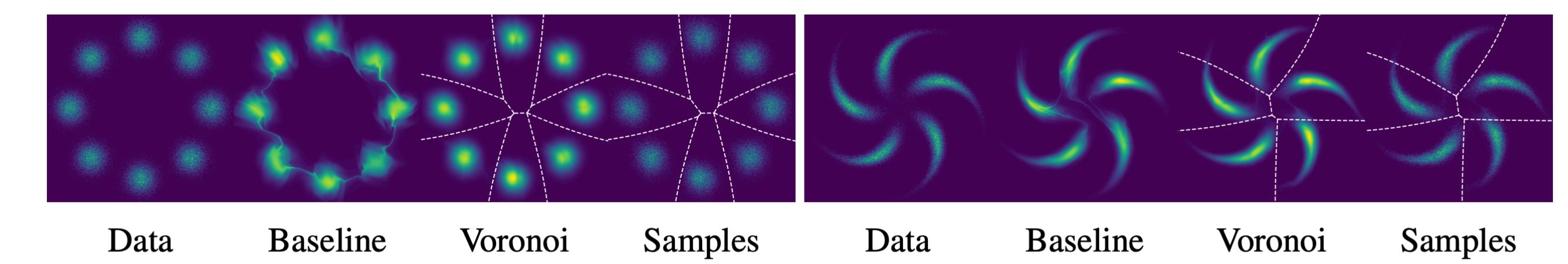


Figure 6: Tessellation is done in a transformed space; nonlinear boundaries are shown.

Table 4: Disjoint mixture modeling. NLL on the test sets in nats. *Baseline results from [13, 35].

Method	POWER	GAS	HEPMASS	MINIBOONE	BSDS300
Real NVP*	-0.17 ± 0.01	-8.33 ± 0.07	18.71 ± 0.01	13.55 ± 0.26	-153.28 ± 0.89
MAF*	-0.24 ± 0.01	-10.08 ± 0.01	17.73 ± 0.01	12.24 ± 0.22	-154.93 ± 0.14
FFJORD*	-0.46 ± 0.01	-8.59 ± 0.12	14.92 ± 0.08	10.43 ± 0.22	-157.40 ± 0.19
Base Coupling Flow	-0.44 ± 0.01	-11.75 ± 0.02	16.78 ± 0.08	10.87 ± 0.06	-155.14 ± 0.04
Voronoi Disjoint Mixture	-0.52 ± 0.01	-12.63 ± 0.05	16.16 ± 0.01	10.24 ± 0.14	-156.59 ± 0.14