QUVA Deep Vision Lab

University of Amsterdam
Faculty of Science

Categorical Normalizing Flows via Continuous Transformations

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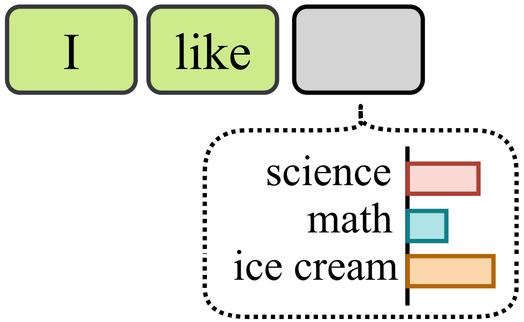
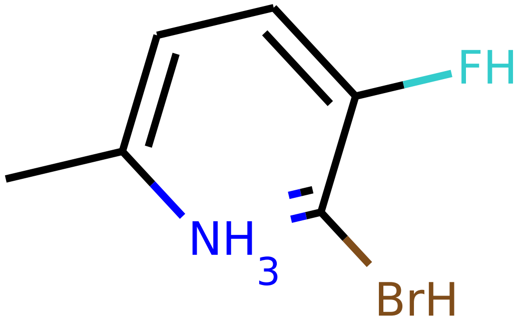
Introduction
Motivation

Categorical Data

Language

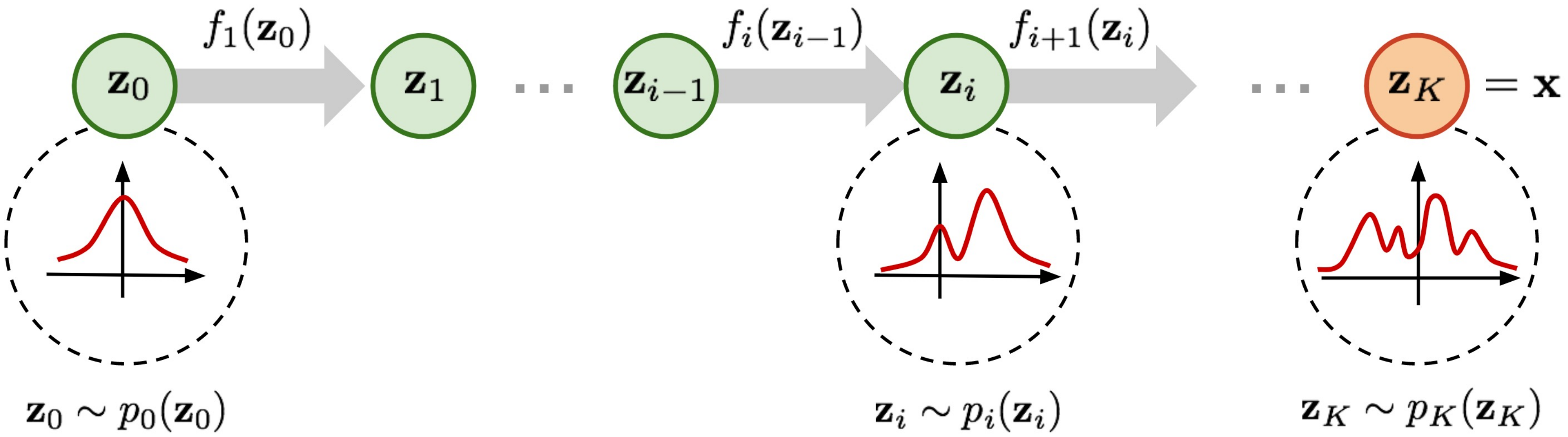


Graphs



Introduction
Preliminaries

Normalizing Flows

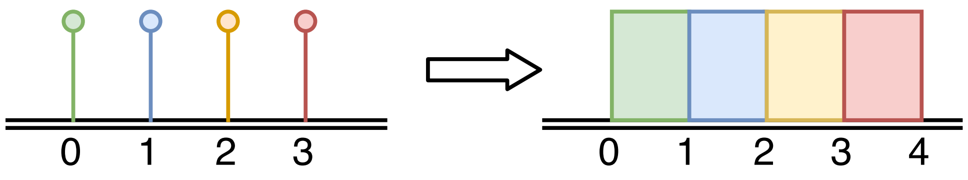


+ Universality
+ Exact likelihood estimate
+ Efficient density evaluation and (parallel) sampling

Figure credit: Weng, Lilian. “Flow-based Deep Generative Models”, 2018.

Introduction
Related Work

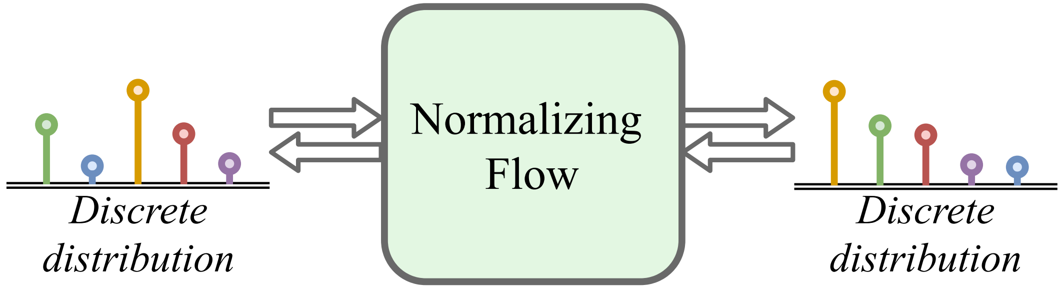
Applying (Variational) Dequantization



Designed for image modeling

– Categories are not "quantized" real values

Discrete Normalizing Flows



– Is limited to permutations

– Not universal with factorized prior

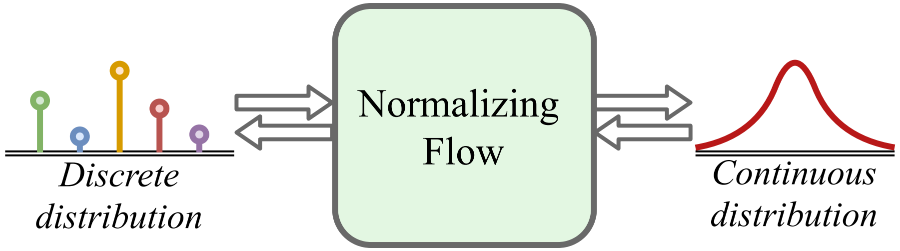
– (Biased) gradient approximations and difficult optimization

References
Tran, D. et al.: "Discrete Flows: Invertible Generative Models of Discrete Data". NeurIPS, 2019.
Hoogeboom, E. et al.: "Integer Discrete Flows and Lossless Compression". NeurIPS, 2019.

Introduction
Contributions

Categorical Normalizing Flow

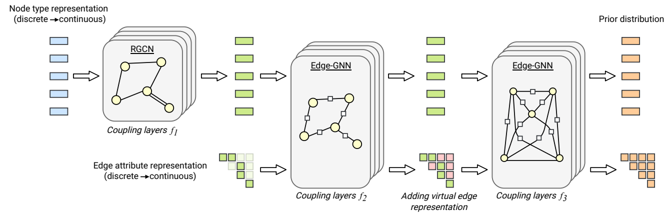
Modeling categorical distribution by a continuous normalizing flow

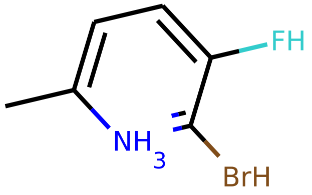


+ Universality
+ Stable optimization without biased gradients
+ Efficient density evaluation and (parallel) sampling

GraphCNF

Powerful graph generation model based on Categorical Normalizing Flows





+ One-shot generation
+ Permutation-invariant to node order
+ Support of categorical node and edge attributes

Categorical Normalizing Flows

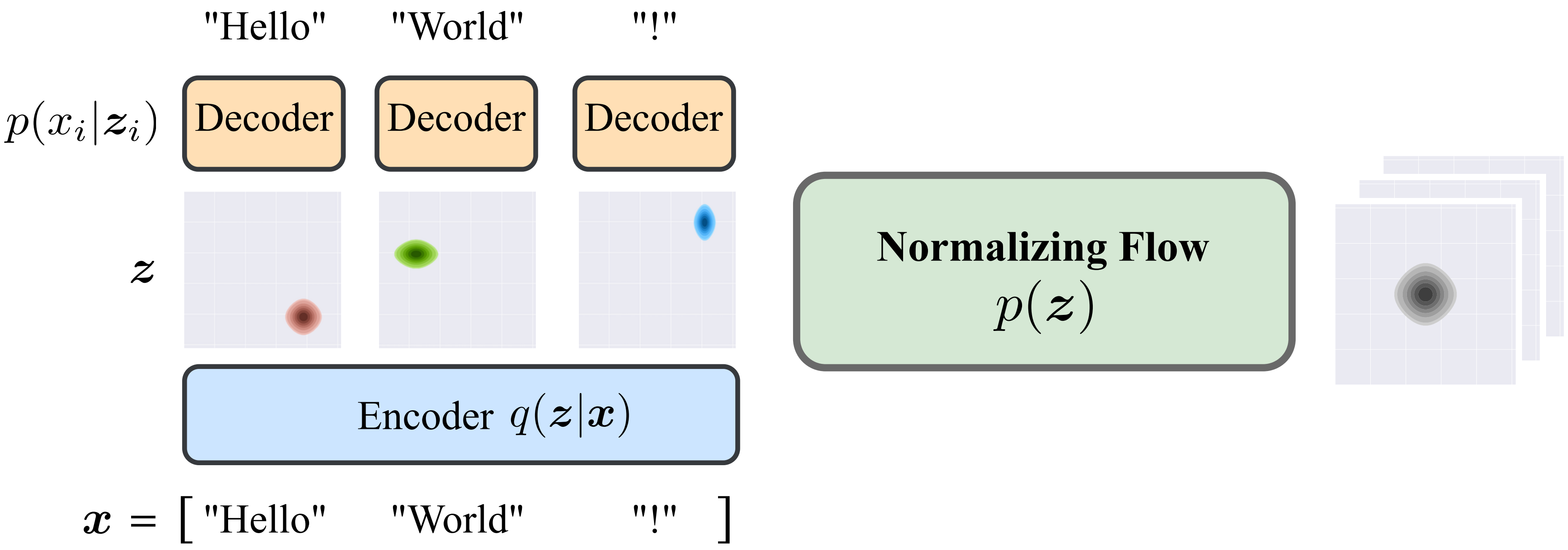
Encoding

- First step: represent categorical data in continuous space
- Desired properties of an encoding function
  - ➜ No loss of information (non-overlapping volumes)
  - ➜ Learnable
  - ➜ Smooth
  - ➜ Support for higher dimensions

⇒ Variational inference with factorized decoder: $p(\boldsymbol{x}) \geq \mathbb{E}_{\boldsymbol{z}\sim q(\cdot|\boldsymbol{x})}\left[\frac{\prod_i p(x_i|\boldsymbol{z}_i)}{q(\boldsymbol{z}|\boldsymbol{x})}p(\boldsymbol{z})\right]$

- Ensures that continuous form z contains the exact same information as discrete x
- ⇒ all model complexity inside the flow

Categorical Normalizing Flows
Overview



Objective function: $p(\boldsymbol{x}) \geq \mathbb{E}_{\boldsymbol{z}\sim q(\cdot|\boldsymbol{x})}\left[\frac{\prod_i p(x_i|\boldsymbol{z}_i)}{q(\boldsymbol{z}|\boldsymbol{x})} p(\boldsymbol{z})\right]$

Categorical Normalizing Flows

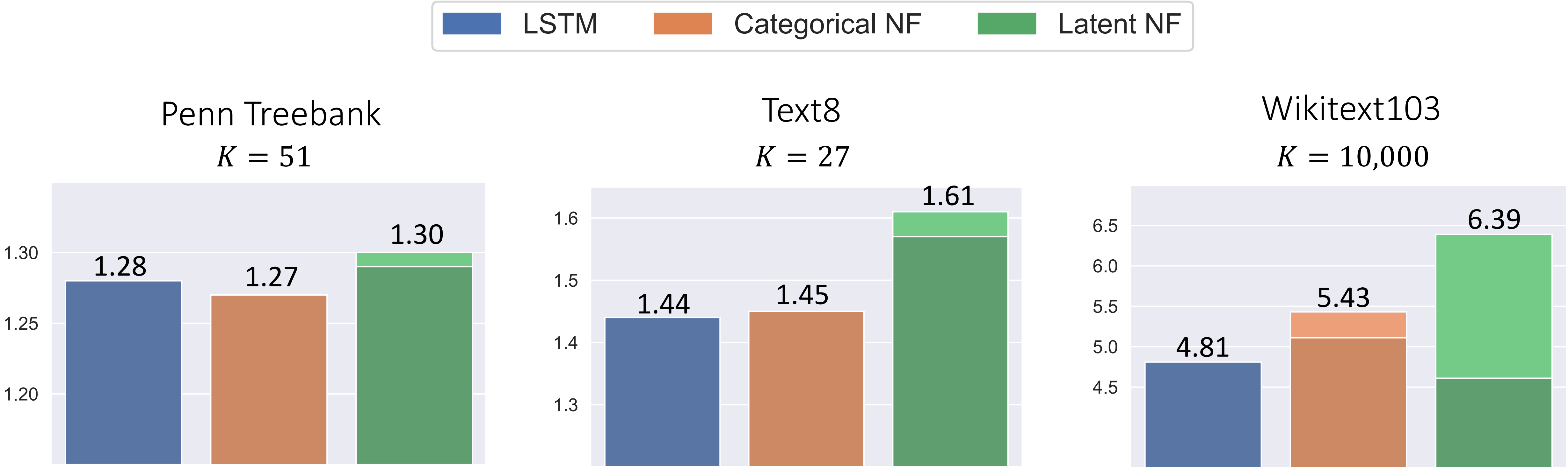
Experiments – Set Modeling

- Toy datasets on sets with known dataset likelihood
- **Metric**: test likelihood in bits per categorical variable (lower = better)

Model	**Set shuffling**	**Set summation**
Discrete NF	3.87 $\pm$0.04	2.51 $\pm$0.00
Variational Dequantization	3.01 $\pm$0.02	2.29 $\pm$0.01
Latent NF	**2.78** $\pm$0.00	2.26 $\pm$0.01
CNF + Mixture model		
CNF + Linear flows		
CNF + Variational Encoding		
Optimal	2.77	2.24

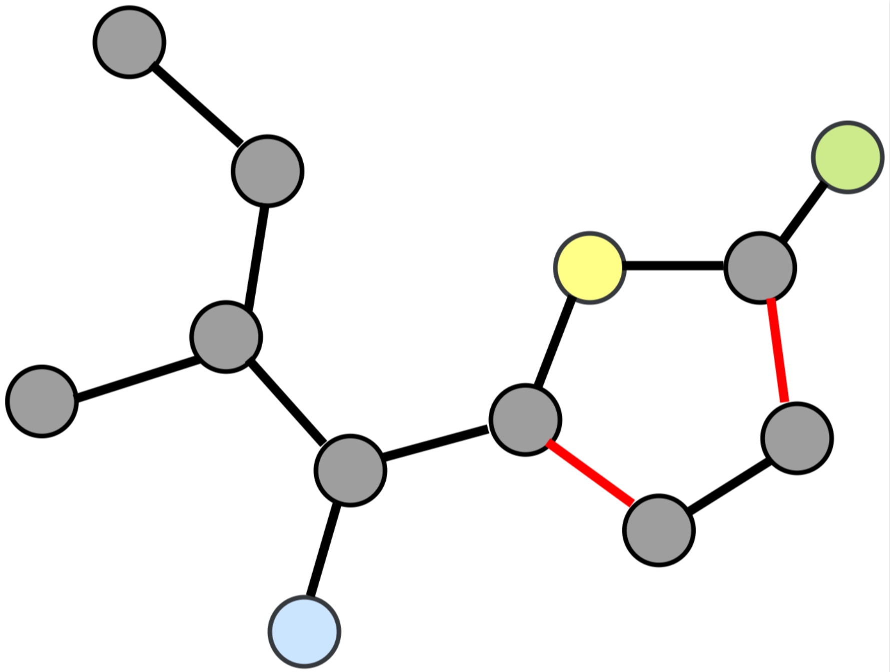
Categorical Normalizing Flows

Experiments – Language Modeling



Metric: bits per character/word

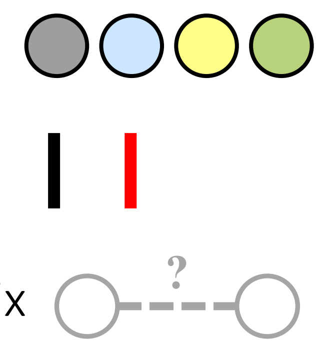
Graph Generation with CNF
Introduction



(1) Node attributes

(2) Edge attributes

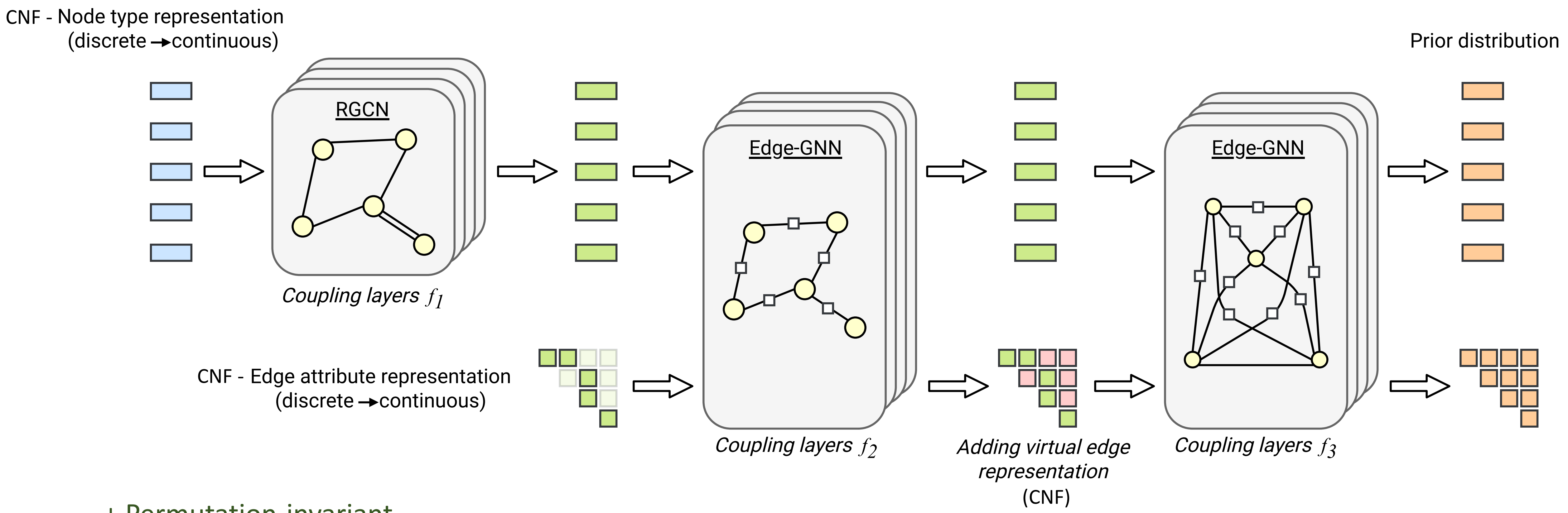
(3) Adjacency matrix



Challenge: nodes are unordered, i.e. a set
⇒ Maintain permutation-invariance of nodes

Graph Generation with CNF

GraphCNF



+ Permutation-invariant
+ Efficient three-step approach

Graph Generation with CNF

Experiments – Molecule Generation

- **Task**: given a set of molecules, learn to model the space of valid molecules
- **Metrics**: calculated on 10k generated graphs,

  (1) Validity: percentage of graphs being valid molecules

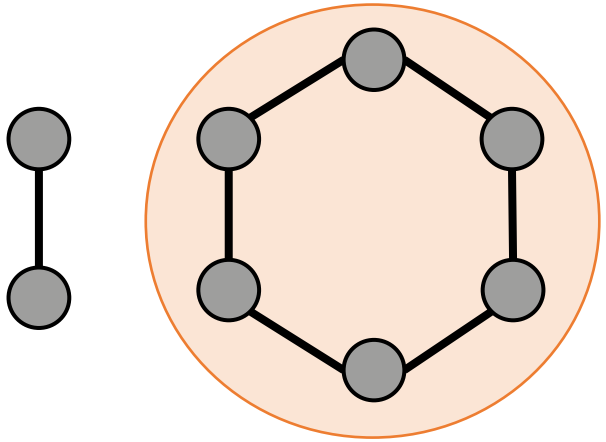
  (2) Uniqueness: percentage of unique molecules

  (3) Novelty: percentage of molecules that are not equal to any training molecule

  (4) Reconstruction: reconstruction accuracy of test molecules from latent space

Graph Generation with CNF

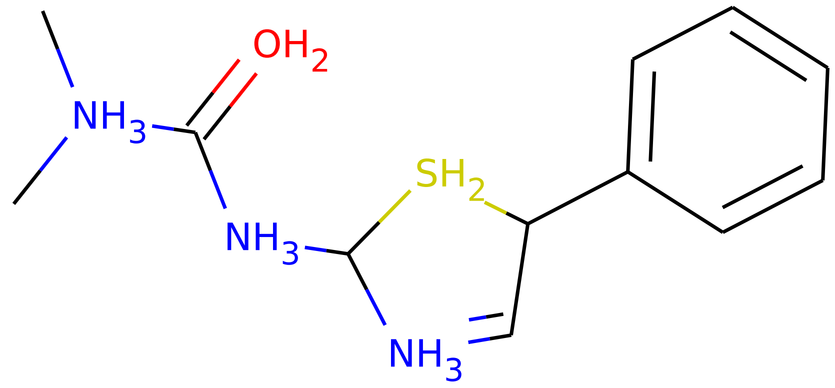
Experiments – Molecule Generation

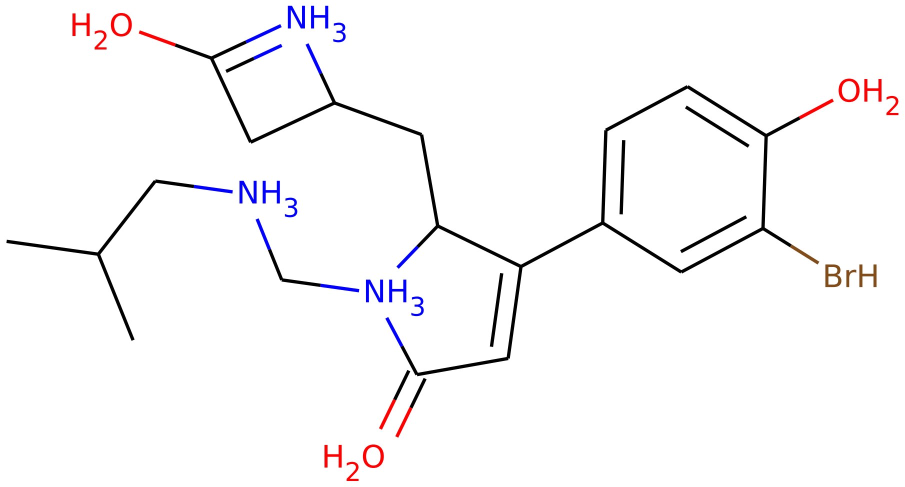


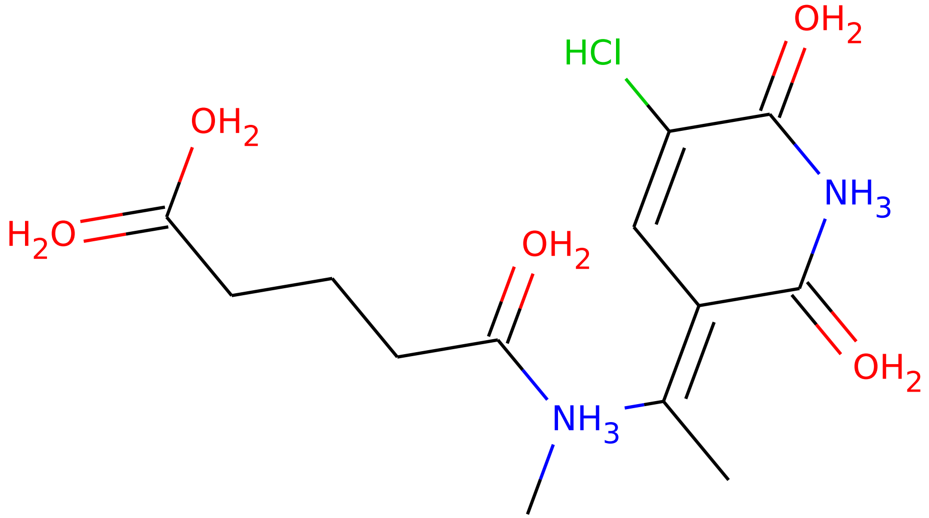
Results on the Zinc250k dataset
(224k examples)

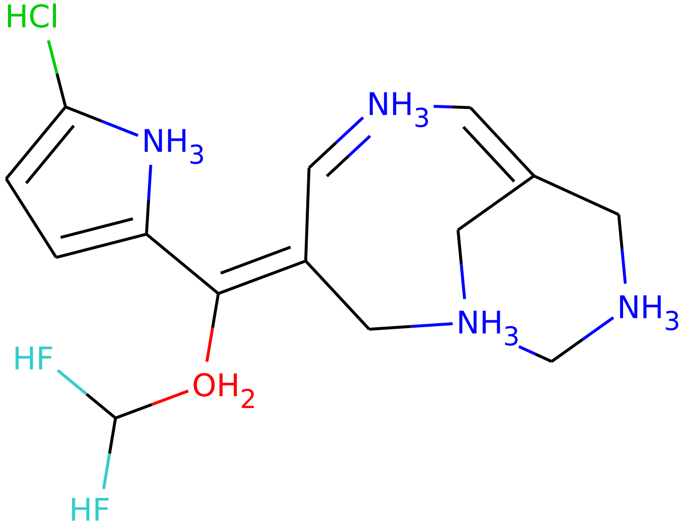
Method	Validity	Uniqueness	Novelty	Reconstruction	Parallel	General
JT-VAE	100%	100%	100%	71%	✗	✗
GraphAF	68%	99.10%	100%	100%	✗	✓
R-VAE	34.9%	100%	–	54.7%	✓	✓
GraphNVP	42.60%	94.80%	100%	100%	✓	✓
GraphCNF	83.41% (± 2.88)	99.99% (± 0.01)	100% (± 0.00)	100% (± 0.00)	✓	✓
+ Sub-graphs						

Graph Generation with CNF
Experiments – Molecule Generation









Conclusion

- Mixture model encoding can be used as “dequantization” for categorical data
  - Simple, efficient, and learnable
- CNFs enable strong, latent-based generative models on domains like graphs
  - GraphCNF significantly outperforms previous flow-based approach on molecule generation
- Possible future direction:
  - Combining continuous and discrete normalizing flows
  - GraphCNF on large graphs ($|V| > 100$)

Thank you. Questions?