Invertible Generative Modeling using Liner Rational Splines

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Abstract

- **Normalizing flows**: modeling arbitrary distributions through invertible mappings
- **Motivation**: investigating other families of invertible functions useful for flow-based modeling
- **Proposal**: monotonic linear rational splines
- **Key features**:
  1. Closed-form inverse
  2. Same family of inverse and forward mappings

Normalizing Flows

Change-of-variables formula:

- Random vector $\mathbf{Z} \sim p_{\mathbf{Z}}(\mathbf{z})$
- Invertible and differentiable function $\mathbf{f}(\cdot)$
- Random vector $\mathbf{X} = \mathbf{f}(\mathbf{Z})$

$$p_{\mathbf{X}}(\mathbf{x}) = p_{\mathbf{Z}}(\mathbf{z}) \left|\det\left(\nabla_{\mathbf{z}}\mathbf{f}(\mathbf{z})\right)\right|^{-1}$$

Normalizing flows:

- $\mathbf{Z}$: simple base random variable (e.g. standard normal)
- $\mathbf{f}_{\boldsymbol{\theta}}(\cdot)$: composition of invertible neural nets

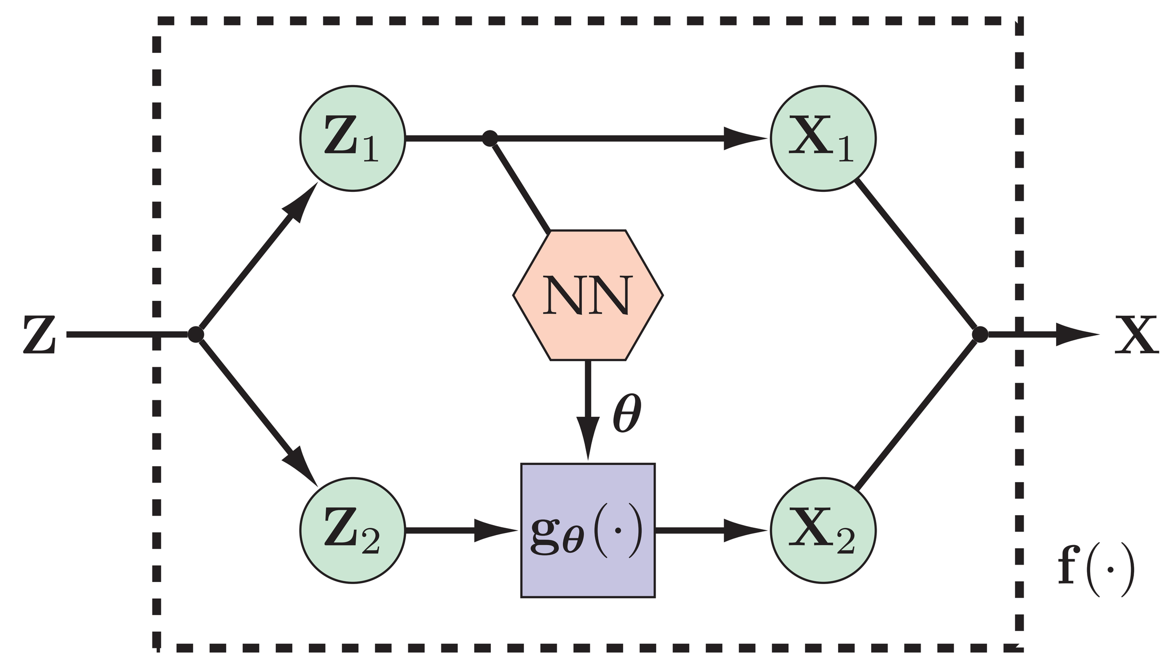
$$\mathbf{f}_{\boldsymbol{\theta}}(\cdot) = \left(\mathbf{f}_K \circ \mathbf{f}_{K-1} \circ \mathbf{f}_2 \circ \mathbf{f}_1\right)(\cdot)$$

- Fitting $\mathbf{f}_{\boldsymbol{\theta}}(\cdot)$ to observations through MLE
- Desirable properties of $\mathbf{f}_{\boldsymbol{\theta}}(\cdot)$:
  1. Tractable $\left|\det\left(\nabla_{\mathbf{z}}\mathbf{f}_{\boldsymbol{\theta}}(\mathbf{z})\right)\right|$
  2. Easily invertible

References

[1] Dinh et al. Density estimation using Real NVP. 2017.
[2] Fuhr and Kallay. Monotone linear rational spline interpolation. 1992.
[3] Durkan et al. Neural spline flows. 2019.

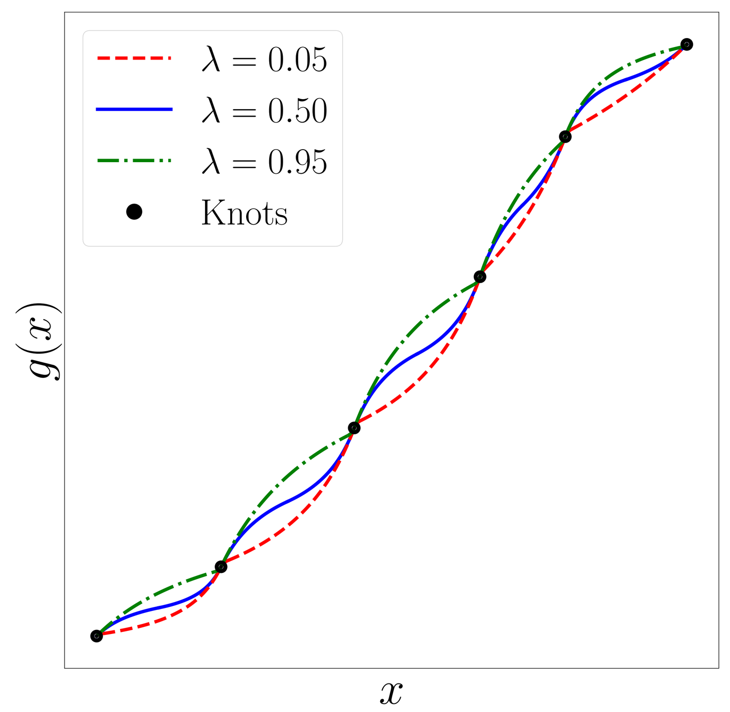
Coupling Layers



- $\mathbf{g}_{\boldsymbol{\theta}}(\cdot)$:
  1. Invertible
  2. Element-wise and differentiable

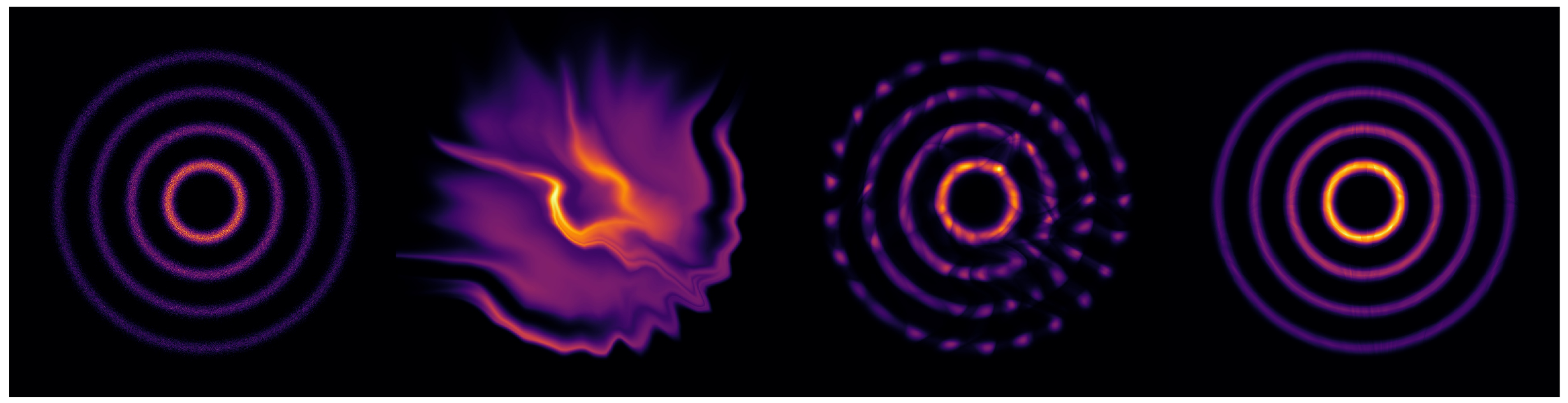
Linear Rational Spline Flow

- **Linear rational splines (LRS)**: piece-wise functions of the form $(ax+b)/(cx+d)$
- **Proposed method**:
  1. Find $\boldsymbol{\theta}$={knot locations, derivative at knot points, λ's (curvature parameters)}
  2. Use the algorithm of [2] for monotonic LRS interpolation and determine the invertible transformarion $\mathbf{g}_{\boldsymbol{\theta}}(\cdot)$.



- **Pros & Cons**:
  - \+ Closed-form inverse.
  - \+ Inverse and forward functions are both LRS.
  - − Slightly (<1%) more number of parameters compared to [3].

Synthetic Density Estimation



Data Samples | Glow | i-ResNet | Ours

Density Estimation of Real-world Data

MODEL	POWER	GAS	HEPMASS	MINIBOONE	BSDS300
FFJORD	0.46	8.59	-14.92	-10.43	157.40
Glow	0.42 ± 0.01	12.24± 0.03	-16.99 ± 0.02	-10.55± 0.45	156.95 ± 0.28
Q-NSF (C)	0.64 ± 0.01	12.80± 0.02	-15.35 ± 0.02	-9.35 ± 0.44	157.65 ± 0.28
RQ-NSF (C)	0.64 ± 0.01	13.09± 0.02	-14.75 ± 0.03	-9.67 ± 0.47	157.54 ± 0.28
Ours (C)	0.65 ± 0.01	12.99 ± 0.02	-14.64 ± 0.03	-9.65 ± 0.48	157.70 ± 0.28

MNIST Image Generation

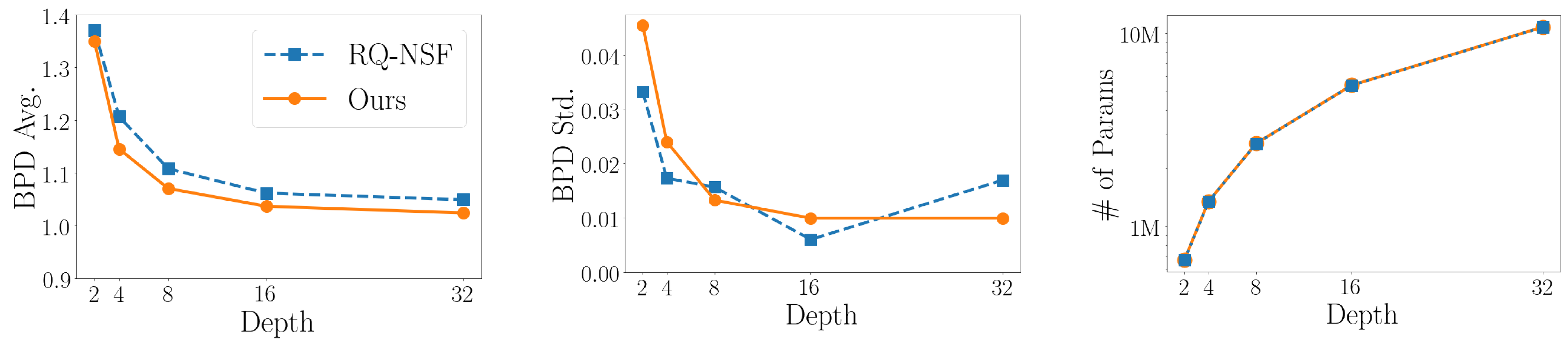
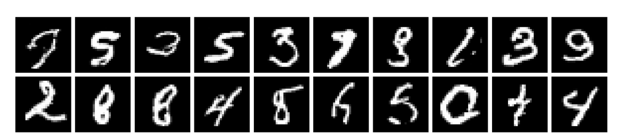
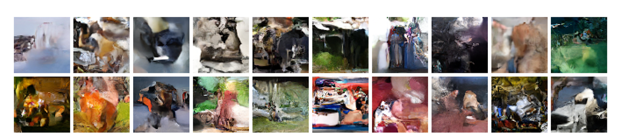


Image Modeling

MODEL	CIFAR-10	IMAGENET 64
Real NVP	3.49	3.98
Glow	3.35	3.81
Residual Flows	3.28	3.75
RQ-NSF (C)	3.38	3.82
Ours (C)	3.38	3.82



MNIST



ImageNet-64

Conclusion

- **LRS**: a family of splines, useful in NF modeling
- **LRS Flows**: closed-form inverse, efficient sampling, competitor of complex existing methods

Contact Information

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