Normalizing flow neural networks by JKO scheme

Chen Xu[1]
joint work with Xiuyuan Cheng[2] and Yao Xie[1]

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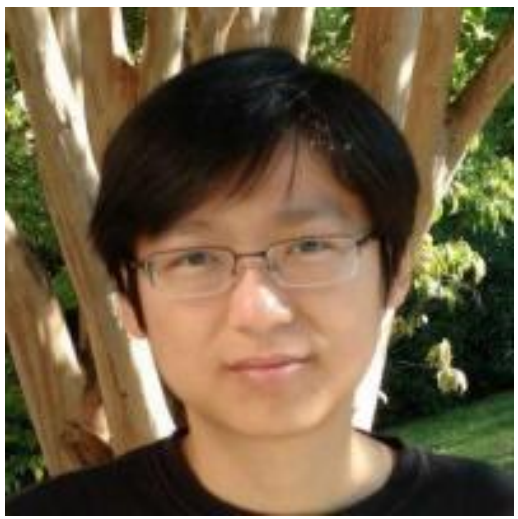
Acknowledgement

• Xu, C., Cheng, X., and Xie, Y. (2022). Normalizing flow neural networks by JKO scheme. *NeurIPS 2023, spotlight.*



(a) Prof. Xiuyuan Cheng

(b) Prof. Yao Xie

Figure 1: My wonderful and supportive collaborator Prof. Xiuyuan Cheng and advisor Prof. Yao Xie

Outline

- Motivation and objective
- Related works
- Proposed method
- Comparison with diffusion models
- Experimental results
- Extensions
- Conclusions

Motivation

- Generative modeling is fundamental in statistics and ML.
  - Statistics: Inferring and sample from the population P_X.
  - Machine learning: Large-language models (e.g., ChatGPT), Image generation (e.g., DALLE-3), etc.

C Skeleton for a good research presentation slide in 5 bullets

Sure, here's a skeleton for a good research presentation slide in 5 bullets:

1. Introduction:
   - Briefly introduce the topic and research question
   - Explain the importance and relevance of the research
2. Objectives:
   - State the research objectives or aims
   - Provide a brief overview of the methods used to achieve the objectives
3. Results:
   - Summarize the main findings of the study
   - Use charts, graphs, tables, or images to present the data
4. Discussion:
   - Interpret the results and explain their significance
   - Discuss the implications of the findings for practice and future research
5. Conclusion:
   - Summarize the key points of the presentation
   - Provide a call-to-action or future directions for research or practice

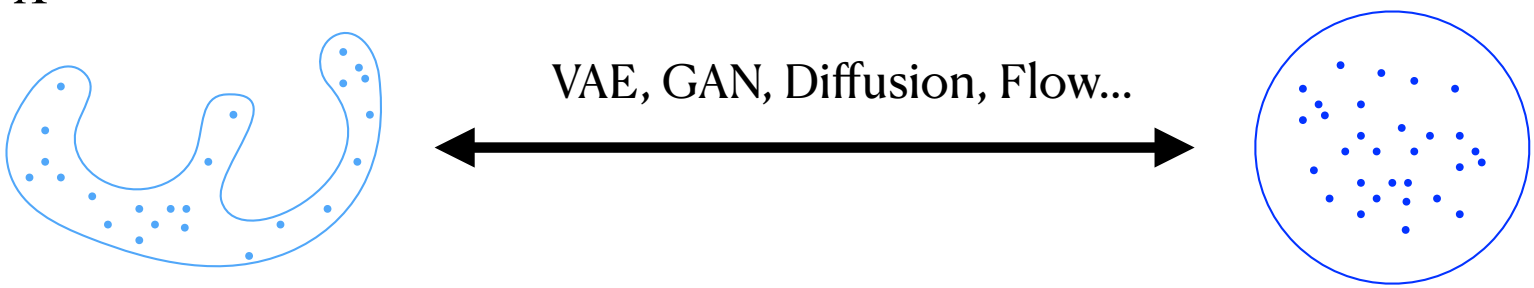
(a) Prompt: "Skeleton for a good research presentation slide in 5 bullets".

(b) Prompt: "A PhD student intently preparing for his research presentation in front of a computer showing the logo GT, cartoon style"

Motivation (cont.)

P_X: Data (Hard)

Z: Noise (Easy)

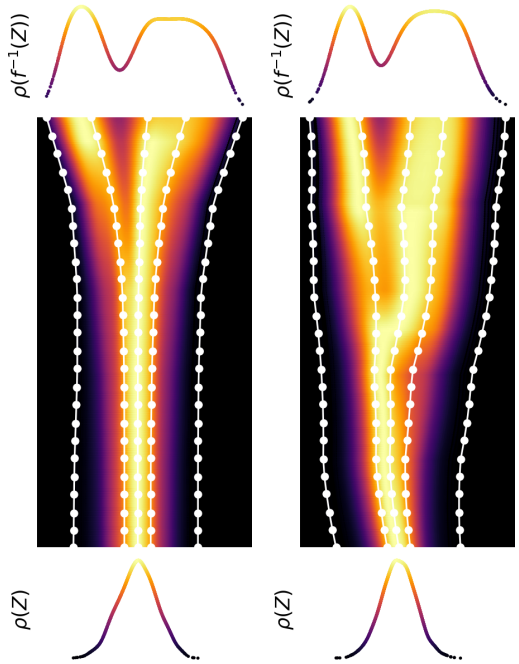


Goal

• Improve the design and training of **normalizing flows**. Namely, invertible transformation of $X \leftrightarrow Z$ given samples from P_X.

• Allow efficient sampling from P_X and likelihood estimation $\log p(X)$.

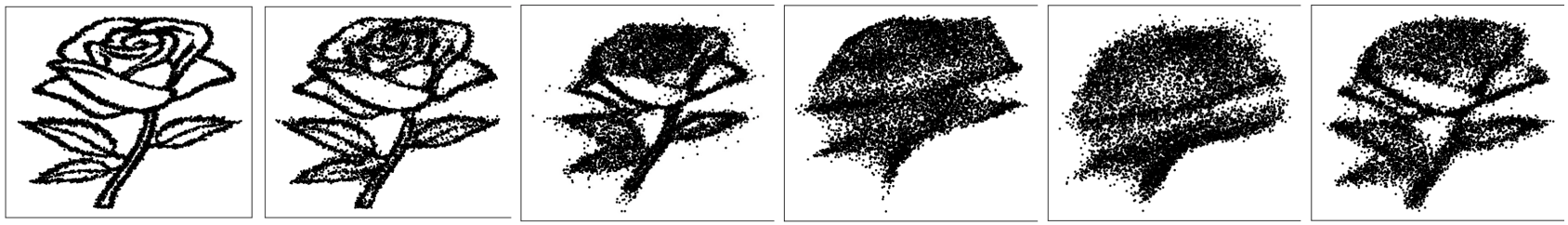
• More computational and memory efficient than existing methods.



(a) JKO-iFlow **(b)** Usual CNF

Figure 1:
$X \leftrightarrow Z, Z \sim \mathcal{N}(0, I_d)$.

Illustration



(a) True data	JKO-iFlow	(b) FFJORD	(c) OT-Flow	(d) IGNN	(e) ScoreSDE
τ: **2.79e-4**, MMD-c:	2.73e-4	3.88e-4	1.42e-3	3.14e–3	6.90e-4
NLL	2.64	2.95	3.30	3.35	3.2

Figure 1: 2D illustration and comparison.

Figure 2: Gradual deformation along $X \leftrightarrow Z$ in the latent space of a VAE.

Related works

- Traditional generative models: Hidden markov models [Baum and Petrie 1966, Rabiner and Juang 1986, Mor et al., 2021], Bayesian network [Heckerman 1996, Koller and Firedman 2009], ...

  Challenges: model assumption and specification, performance in high dimension.

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- Deep Generative models using neural networks (NN): GAN [Goodfellow et al., 2014, Mirza and Osindero 2015, Gulrajani et al., 2017, ...], VAE [Kingma and Welling 2014, 2019, ...]

  Challenges: mode collapse and vanishing gradients [Salimans et al., 2016], posterior collapse [Lucas et al., 2019], and so on. Neither GAN nor VAE provides explicit data density.

Related works (cont.)

- Normalizing flow models: FFJORD [Grathwohl et al., 2019], graph flow [Liu et al., 2019], OT-Flow [Onken et al., 2021]...

  Challenges: computation and memory efficiency, model regularization.

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  Challenges: computation and memory efficiency, model regularization.

- Neural SDE-based: score-based generative models [Song and Ermon, 2019, Song et al., 2021, Boffi & Vanden-Eijnden, 2022],

  Challenges: efficient and accurate sampling of SDE trajectory, difficulty in learning the score at all $t \in [0, T]$ with small networks.

Mathematical background

- Normalizing flow: density evolution of $\rho(x,t)$, with $\rho(x,0) = p_X$ and $\lim_{t\to\infty} \rho(x,t) = p_Z \sim \mathcal{N}(0, I_d)$.

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  - Liouville equation: $\partial_t \rho + \nabla \cdot (\rho f) = 0$.
  - Example: (multivariate) Ornstein-Uhlenbeck (OU) process with the Fokker-Planck equation describing $\rho(x,t)$ to p_Z.

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- Transport regularization: $\mathcal{T} = \int_0^1 \mathbb{E}_{x\sim\rho(\cdot,t)} \|f(x,t)\|^2 dt$.
  - Recovers the Wasserstein-2 optimal transport under the Benamou-Brenier formula [Villani 2009]).

Mathematical background (cont.)

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- Normalizing flow models learn f using neural networks f_θ.
- Specifically, the objective is

$$\min_\theta \mathrm{KL}((T_\theta)_{\#} p_X || p_Z) + \mathcal{R}(\theta). \tag{2}$$

- $T_\theta(x) = x + \int_0^1 f_\theta(x(s), s), x(0) = x$;
  $T_{\#}$ is the push-forward operation with $(T_{\#} p)(A) = p(T^{-1}(A))$ for a measureable set A.

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- (2) is equivalent to maximizing $\log p(X)$ up to constants [Onken et al., 2021].

Current approaches

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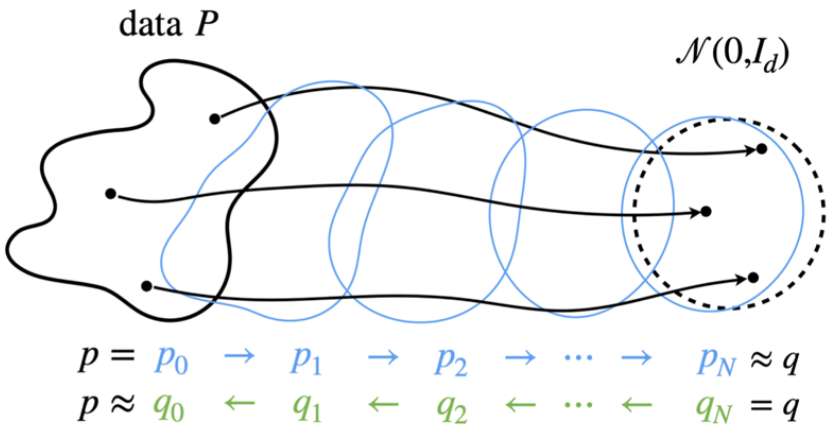
  - Namely, the integral from $[0, 1]$ is broken into a sequence of L smaller integrals each with f_{θ_l}, or the model f_θ itself is a composition of L smaller ones of identical architecture.
- Challenges are
  - Design: how to specify L.
  - Computation: joint training of all L blocks.
  - Memory: samples are passed through all L blocks.

Main contribution

- Introduce block-wise training of CNF models, where each block is allowed simpler architecture.
- Efficient training with less computation and memory cost.
- Better generative performance and likelihood estimation vs CNF and diffusion models on simulated and real data.

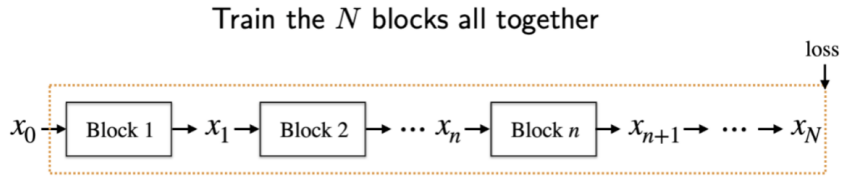
Proposed JKO-iFlow (informal)

- Conceptual understanding

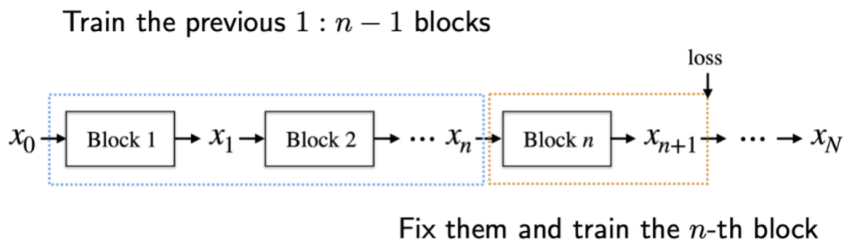


- Practical implication

- Existing end-to-end training



- Our progressive training



Proposed JKO-iFlow (formal)

- Our JKO-iFlow is inspired by the Jordan-Kinderleherer-Otto (JKO) scheme [Jordan et al., 1998]: starting at $p_0 = \rho_0 \in \mathcal{P}$, with step size $h_k > 0$, the JKO scheme at the $k-$th step is

$$p_{k+1} = \arg\min_{p \in \mathcal{P}} \mathsf{KL}(\rho \| p_Z) + \frac{1}{2h_k} W_2^2(p_k, \rho). \tag{1}$$

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- Theoretical analyses of solving (1) are further studied in [Cheng et al., 2023], including convergence rates of the "forward process" and the data generation guarantee for "backward process'.

[Cheng et al., 2023] Convergence of flow-based generative models via proximal gradient descent in Wasserstein space.

Proposed JKO-iFlow (cont.)

- Let k-th block $T_{\theta_k}(x) = x + \int_0^1 f_{\theta_k}(x(s), s)$ with parameters θ_k.

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- Using the instantaneous change-of-variable formula [Chen et al., 2018], we can show that up to constants

$$\mathsf{KL}((T_{\theta_k})_{\#}p_k \| p_Z) = \mathbb{E}_{x\sim p_k}\left[\|T_{\theta_k}(x)\|^2 - \int_0^1 \nabla \cdot f_{\theta_k}(x(s), s)ds\right].$$

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- Thus, we train the k-th block given the trained $(k-1)$-th block.
- The full model $T_\theta = T_{\theta_K} \circ \ldots \circ T_{\theta_1}$, where $(T_\theta)_{\#}p_X \approx \mathcal{N}(0, I_d)$.

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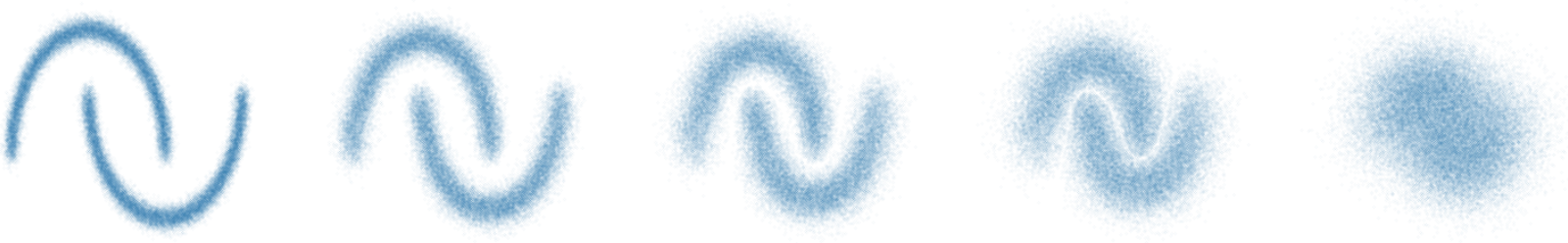

Figure 3: Toy example with 4 trained blocks. X = two moons.

Proposed JKO-iFlow (cont.)

- Computation:
  - The numerical integration is done via fixed-stage Runge-Kutta-4.
  - Finite-difference divergence estimation based on the Hutchinson trace estimator [Hutchinson 1989]:

$$\nabla \cdot f(x,t) \approx \mathbb{E}_{p(\epsilon)}\left[\epsilon^T \frac{f(x+\sigma\epsilon,t)-f(x,t)}{\sigma}\right]$$

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  - Back-propagation uses the adjoint sensitivity method [Pontryagin et al., 1962] implemented in NeuralODE [Chen et al., 2019].
- Benefits:
  - Simpler design and easier training of f_{θ_k}.
  - Allow stopping criterion to determine number of blocks.
  - No sampling (e.g., SDE-based score matching [Song et al., 2021]) nor variational learning (e.g., min-max formulation [Fan et al., 2021]).

Computational techniques

- We further proposed two techniques to improve training and performance. In short,
  - *Reparametrization* adjusts the penalty term h_k to encourage more even W_2 block movements, due to exponential convergence by JKO theory.

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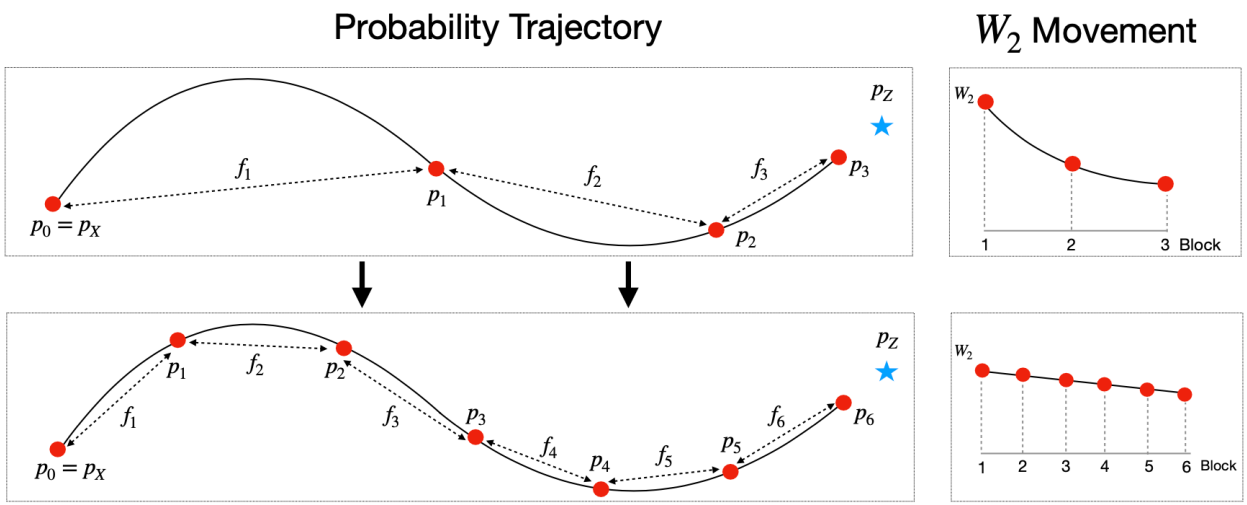

Figure 1: Before and after reparametrization and refinement.

Comparison with diffusion models

- ODE, e.g., JKO flow
- **Particles** $x_0 \sim p$, push particles by velocity field $v(\cdot, t) : \mathbb{R}^d \to \mathbb{R}^d$

$$\dot{x}_t = v(x_t, t)$$

- **Distribution**: Continuity equation $X_t \sim \rho_t$

$$\partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0.$$

- SDE, score matching
- **Noisy samples** $X_0 \sim P$, sample noisy trajectory

$$dX_t = -\nabla V(X_t)dt + \sqrt{2}dW_t$$

- **Distribution**: Fokker-Plank equation $X_t \sim \rho_t$

$$\partial_t \rho_t = \nabla \cdot (\rho_t \nabla V + \nabla \rho_t)$$

Same when setting $v(x, t) = -\nabla V(x) - \nabla \log \rho_t$ "score function"

Comparison with diffusion models (cont.)

- JKO-iFlow
  - **Strength:**

    (·) Training: no noise sampling + flexibility and adaptiveness.

    (·) Inference: direct likelihood estimation.
  - **Limitation:** scalability due to the use of neural ODE in training.

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  - **Limitation:** scalability due to the use of neural ODE in training.
- Diffusion model
  - **Strength:**

    (·) Training: faster in general.

    (·) Inference: superior generative performance on visual tasks.
  - **Limitation:**

    (·) Training: architecture is fixed.

    (·) Inference: indirect likelihood estimation whose accuracy heavily depends on learnt score

Experiments–simulation

- Baselines: two discrete-time flow [Berhmann et al., 2019, Xu et al., 2022], two continuous-time flow [Grathwohl et al., 2019, Onken et al., 2021], and one diffusion model [Song et al., 2021].

- **Takeaway:** JKO-iFlow shows better likelihood estimation and generative performance.

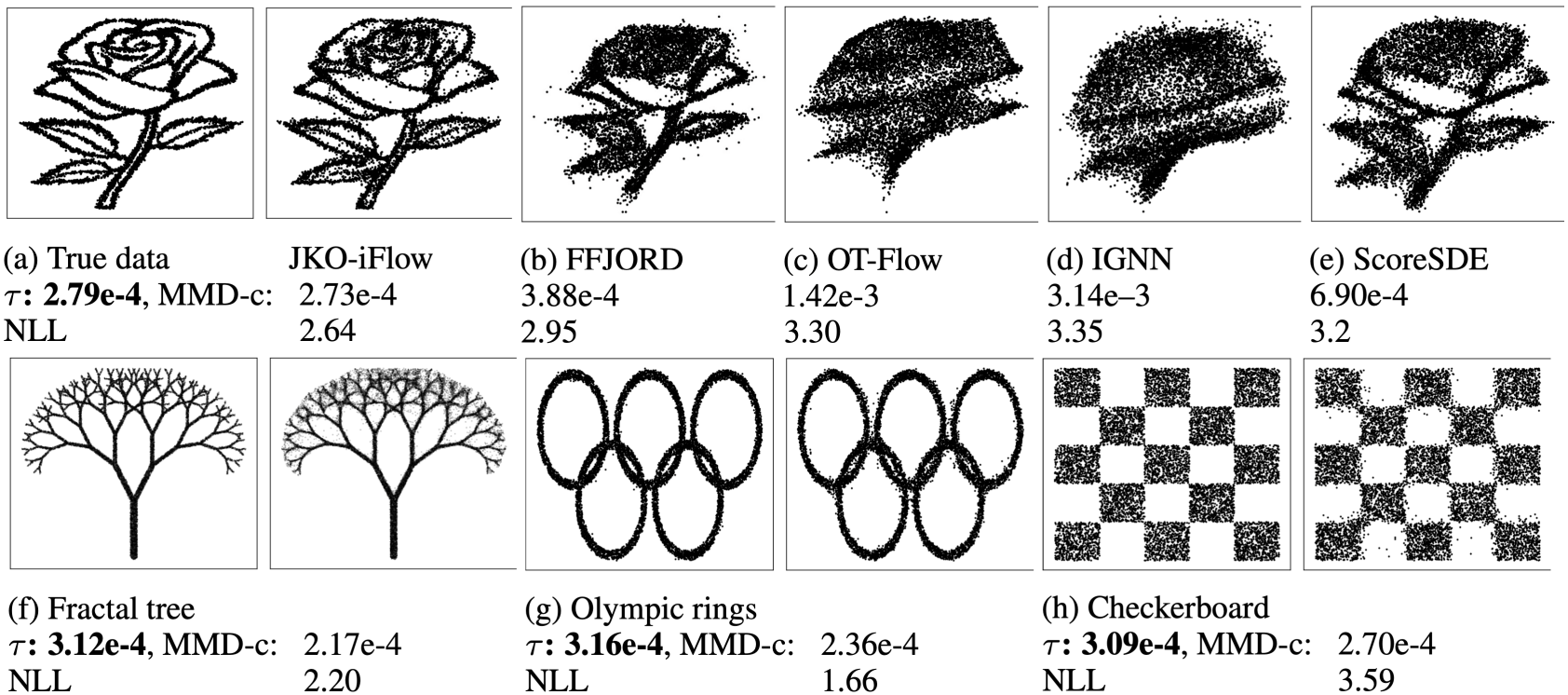
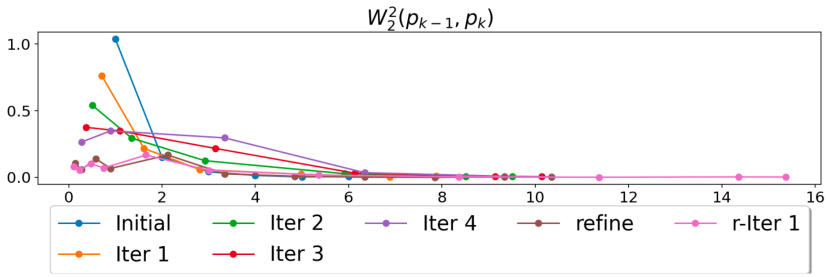


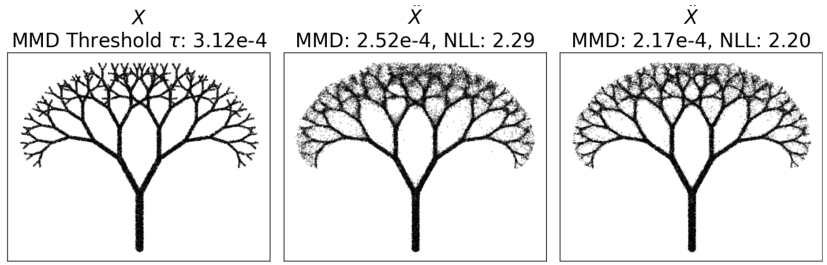
Figure 1: Two-dimensional datasets visualized as scatter plots.

Experiments–simulation (cont.)

- Benefits of reparametrization + refinement.
- **Takeaway:** improved performance on edges, at which we have few samples.



(a) Per-block W_2^2 over reparameterization iterations and refinement ('r-Iter 1' means one reparameterization iteration after refinement).



(b) Results at Iter 4 (middle) and r-Iter 1 (right). MMD and NLL values are shown in the title.

Figure 1: W_2 movement before and after reprametrization and refinement, as well as the generated samples.

Experiments–real data

- High-dimensional tabular datasets ($d = 6, 8, 43, 63$).
- **Takeaway:** competitive or better performance under much less number of mini-batch SGD.

Data Set	Model	# Param	Training				Testing		
			Time (h)	# Batches	Time/Batches (s)	Batch size	MMD-m	MMD-1	NLL
							τ: **1.73e-4**	τ: **2.90e-4**	
POWER $d = 6$	JKO-iFlow	76K, L=4	0.07	0.76K	3.51e-1	10000	9.86e-5	2.40e-4	-0.12
	OT-Flow	76K	0.36	7.58K	1.71e-1	10000	7.58e-4	5.35e-4	0.32
	FFJORD	76K, L=4	0.67	7.58K	3.18e-1	10000	9.89e-4	1.16e-3	0.63
	IGNN	304K, L=16	0.29	7.58K	1.38e-1	10000	1.93e-3	1.59e-3	0.95
	IResNet	304K, L=16	0.41	7.58K	1.95e-1	10000	3.92e-3	2.43e-2	3.37
	ScoreSDE	76K	0.06	7.58K	2.85e-2	10000	9.12e-4	6.08e-3	3.41
	ScoreSDE	76K	0.60	75.80K	2.85e-2	10000	7.12e-4	5.04e-3	3.33
	JKO-iFlow	57K, L=3	0.05	0.76K	2.63e-1	10000	3.86e-4	7.20e-4	-0.06
							τ: **1.85e-4**	τ: **2.73e-4**	
GAS $d = 8$	JKO-iFlow	76K, L=4	0.07	0.76K	3.32e-1	5000	1.52e-4	5.00e-4	-7.65
	OT-Flow	76K	0.23	7.60K	1.09e-1	5000	1.99e-4	5.16e-4	-6.04
	FFJORD	76K, L=4	0.65	7.60K	3.08e-1	5000	1.87e-3	3.28e-3	-2.65
	IGNN	304K, L=16	0.34	7.60K	1.61e-1	5000	6.74e-3	1.43e-2	-1.65
	IResNet	304K, L=16	0.46	7.60K	2.18e-1	5000	3.20e-3	2.73e-2	-1.17
	ScoreSDE	76K	0.03	7.60K	1.42e-2	5000	1.05e-3	8.36e-4	-3.69
	ScoreSDE	76K	0.30	76.00K	1.42e-2	5000	2.23e-4	3.38e-4	-5.58
	JKO-iFlow	95K, L=5	0.09	0.76K	4.15e-1	5000	1.51e-4	3.77e-4	-7.80
							τ: **2.46e-4**	τ: **3.75e-4**	
MINIBOONE $d = 43$	JKO-iFlow	112K, L=4	0.03	0.34K	3.61e-1	2000	9.66e-4	3.79e-4	12.55
	OT-Flow	112K	0.21	3.39K	2.23e-1	2000	6.58e-4	3.79e-4	11.44
	FFJORD	112K, L=4	0.28	3.39K	2.97e-1	2000	3.51e-3	4.12e-4	23.77
	IGNN	448K, L=16	0.63	3.39K	6.69e-1	2000	1.21e-2	4.01e-4	26.45
	IResNet	448K, L=16	0.71	3.39K	7.54e-1	2000	2.13e-3	4.16e-4	22.36
	ScoreSDE	112K	0.01	3.39K	6.37e-3	2000	5.86e-1	4.33e-4	27.38
	ScoreSDE	112K	0.10	33.90K	6.37e-3	2000	4.17e-3	3.87e-4	20.70
							τ: **1.38e-4**	τ: **1.01e-4**	
BSDS300 $d = 63$	JKO-iFlow	396K, L=4	0.05	1.03K	1.85e-1	1000	2.24e-4	1.91e-4	-153.82
	OT-Flow	396K	0.62	10.29K	2.17e-1	1000	5.43e-1	6.49e-1	-104.62
	FFJORD	396K, L=4	0.54	10.29K	1.89e-1	1000	5.60e-1	6.76e-1	-37.80
	IGNN	990K, L=10	1.71	10.29K	5.98e-1	1000	5.64e-1	6.86e-1	-37.68
	IResNet	990K, L=10	2.05	10.29K	7.17e-1	1000	5.50e-1	5.50e-1	-33.11
	ScoreSDE	396K	0.01	10.29K	3.50e-3	1000	5.61e-1	6.60e-1	-7.55
	ScoreSDE	396K	0.10	102.90K	3.50e-3	1000	5.61e-1	6.62e-1	-7.31
	JKO-iFlow	396K, L=4	0.08	1.03K	2.76e-1	5000	1.41e-4	8.83e-5	-156.68

Figure 1: Quantitative metrics (MMD and NLL)

Experiments–real data (cont.)

- High-dimensional tabular datasets ($d = 6, 8, 43, 63$).
- **Takeaway:** A closer visual match between generated and true samples.

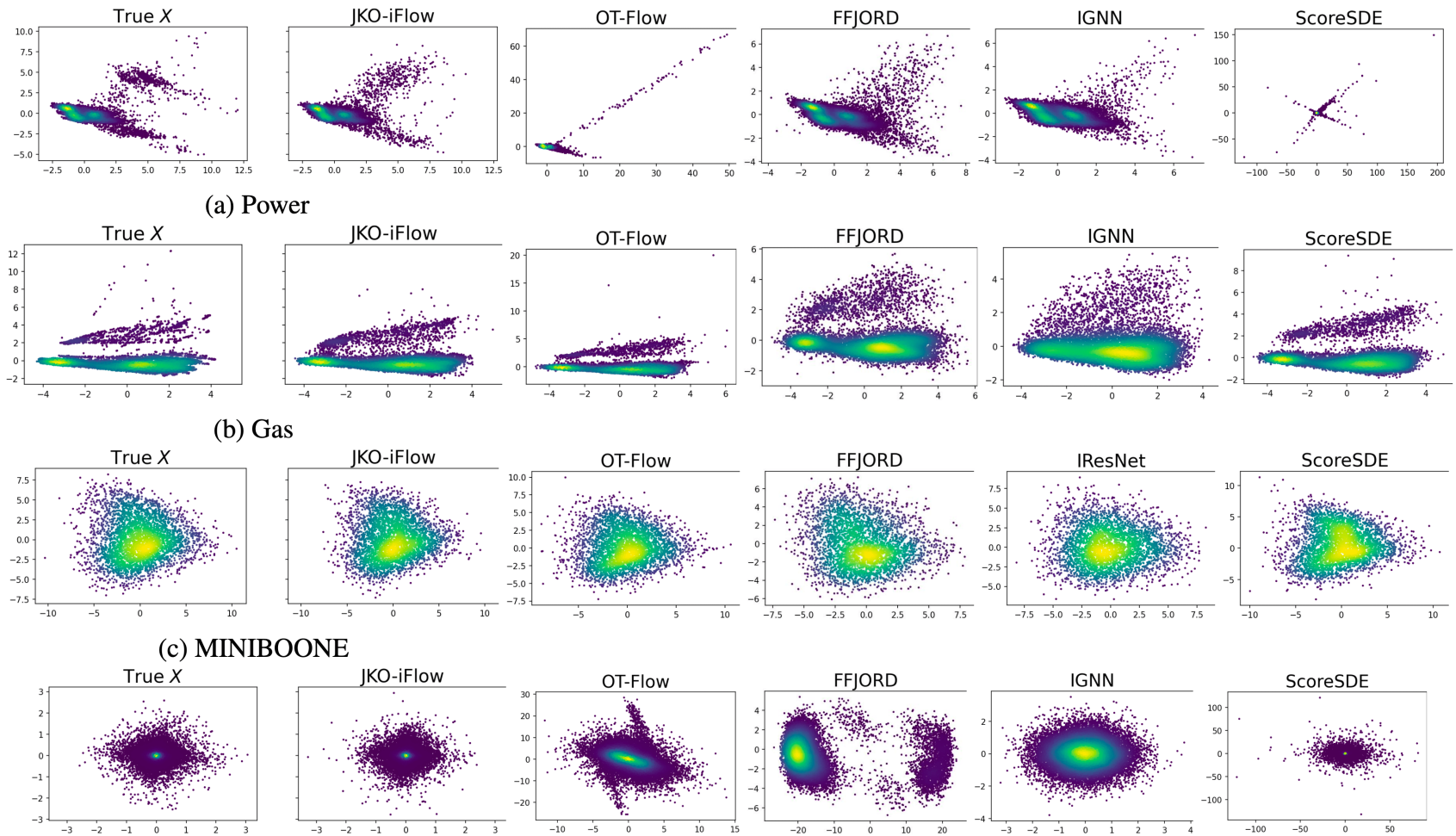


Figure 1: Four real datasets: PCA visualization

Experiments–real data (cont.)

- Performance on tabular data ($d = 43$) without fixed budget.
- **Takeaway:** JKO-iFlow reaches near SOTA performance under much smaller models and training.
  - ScoreSDE has 830K parameters and is trained 100K batches.

Data Set	Model	# Param	Training		Testing
			# Batches	Batch size	NLL
MINIBOONE $d = 43$	JKO-iFlow	112K, L=4	2.72K	2000	10.55
	OT-Flow*	78K	7K	2000	10.55
	FFJORD*	821K, L=1	-	1000	10.43

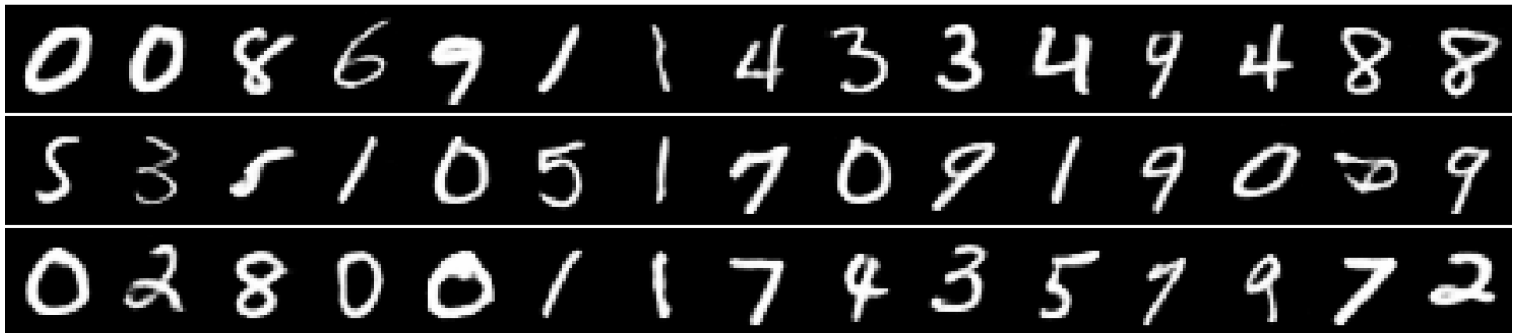
(a) CNF performance

Noise scheduler \ $\beta_{\max}$	5	10	15
Linear	11.33 (0.44)	10.84 (1.17)	10.47 (0.13)
Quadratic	12.88 (0.40)	11.11 (0.24)	11.05 (0.49)

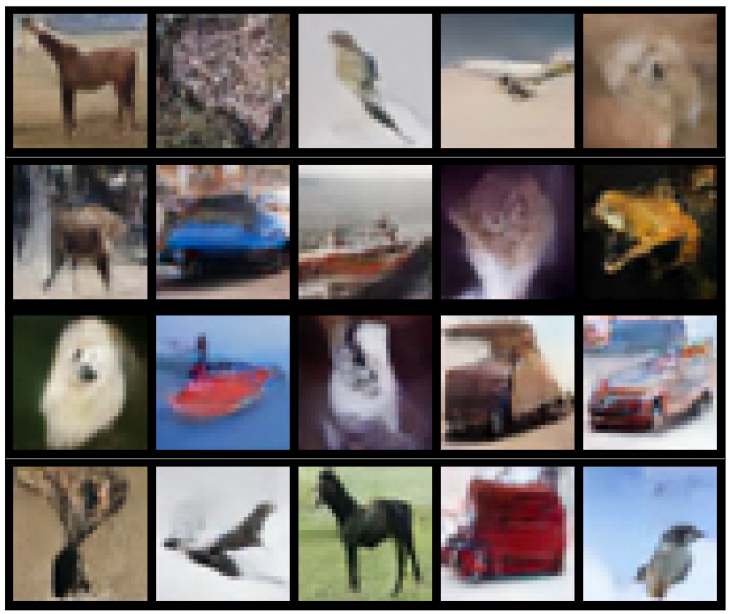
(b) ScoreSDE performance (different noise schedulers)

Experiments–real data (cont.)

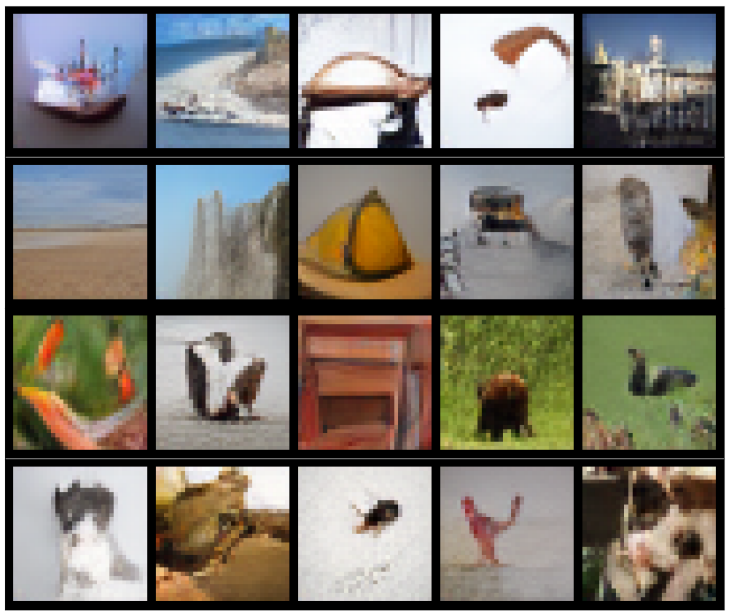
- Image data in the latent space of pre-trained variational auto-encoders [Esser et al., 2021].



(a) Generated MNIST digits. FID: 7.95.



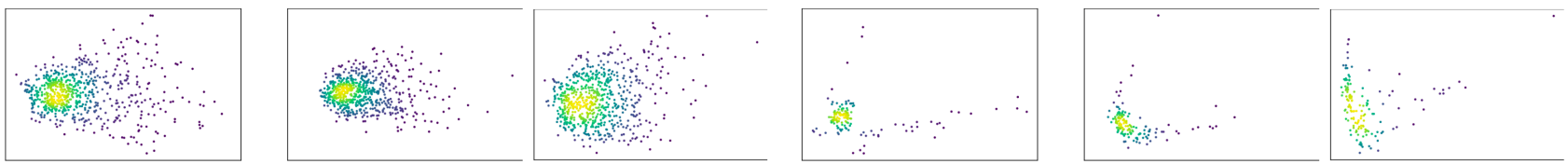
(b) Generated CIFAR10 images. FID: 29.10.



(c) Generated Imagenet-32 images. FID: 20.10.

Experiments–real data (cont.)

- Solar ramping event used in iGNN [Xu et al., 2022], a task of *conditional* generation on graph.
- **Takeaway:** Improved performance by JKO-iFlow in terms of lower NLL and MMD.



(a) True $X\|Y$	JKO-iFlow	(b) IGNN	(c) True $X\|Y$	JKO-iFlow	(d) IGNN
τ: **1.78e-3**, MMD-m:	2.42e-2	3.25e-2	τ: **7.96e-3,** MMD-m:	5.79e-2	9.71e-2
NLL	-0.32	2.46	NLL	-8.75	-3.80

Figure 1: PCA projection and quantitative metrics.

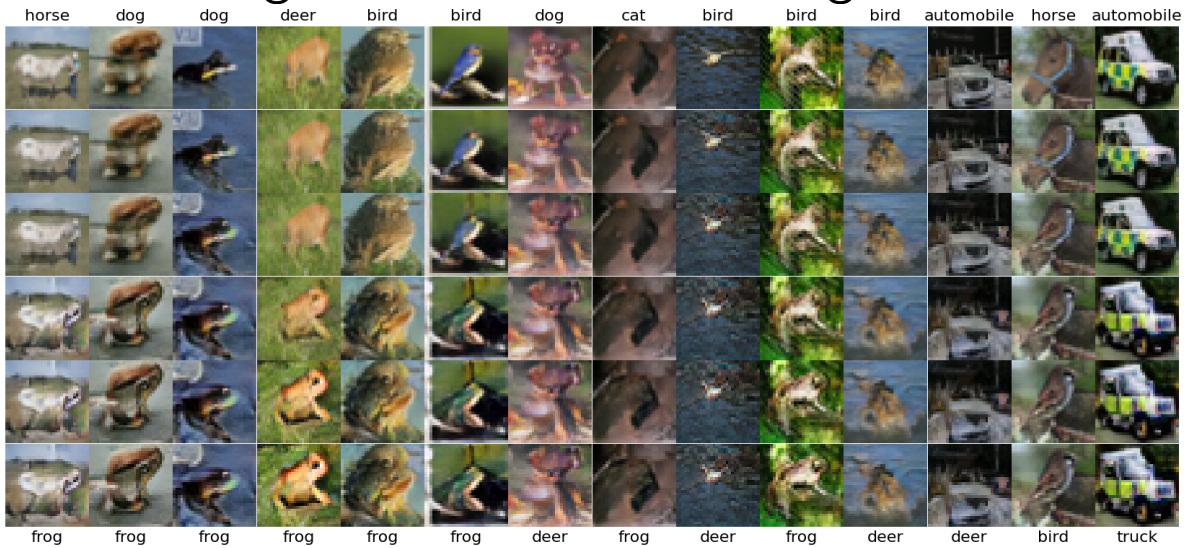
Extension 1: Learn dynamic OT

• We have leveraged flow models in learning high-dimensional optimal transport between arbitrary distributions P and Q; useful for density ratio estimation, image-to-image translation, and so on.

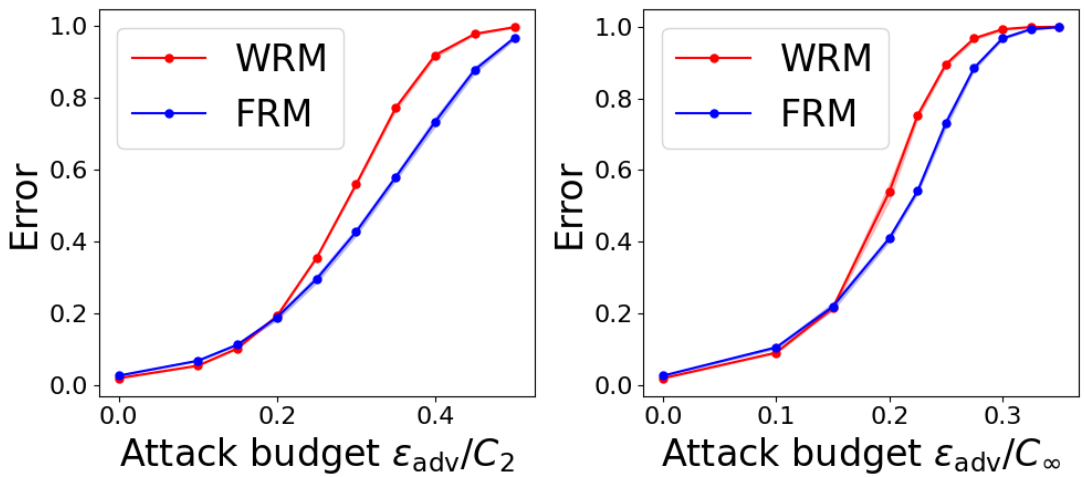
C. Xu, X. Cheng, and Y. Xie, "Computing high-dimensional optimal transport by flow neural networks", arXiv preprint arXiv:2305.11857, 2023

Extension 2: Distributionally robust optimization

- We leveraged the proposed JKO-iFlow to find the worst-case distribution in DRO, where the target distribution is no longer Gaussian $\mathcal{N}(0, I_d)$.



Classification error under PGD attack



C. Xu, J. Lee, X. Cheng, and Y. Xie, "Flow-based Distributionally Robust Optimization", IEEE Journal on Selected Areas in Information Theory (JSAIT), 2024

Conclusions

- Propose JKO-iFlow, a neural ODE model that trains each residual block in a step-wise fashion.
- Leads to improved performance with less computation against flow and diffusion models.
- The flow-based approach has been extended to conditional generation, computing high-dimensional optimal transport, and distributionally robust optimization.

Xu, C., Cheng, X., and Xie, Y. (2022). Normalizing flow neural networks by JKO scheme. *NeurIPS 2023, spotlight.*