Generative Modeling by Estimating Gradients of the Data Distribution

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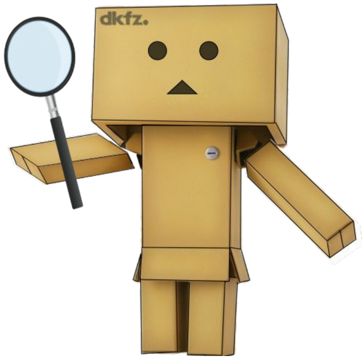
Medical Image Analysis（#MIA-san-mia）
DKFZ



Generative modeling

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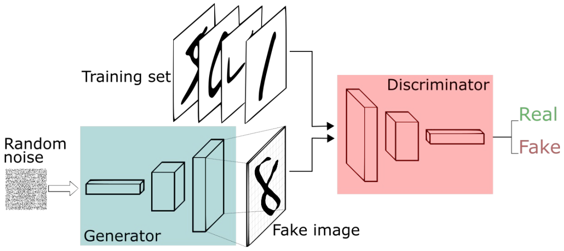
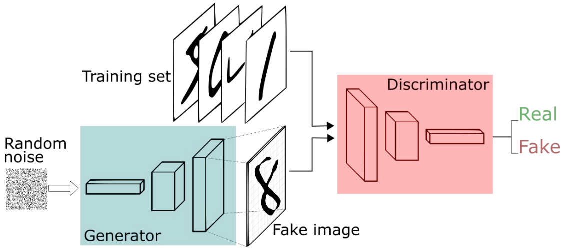


GANs

Generative modeling



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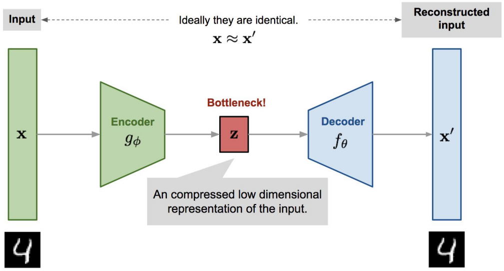
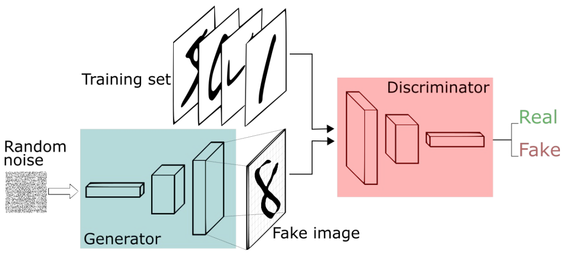


VAEs

Generative modeling



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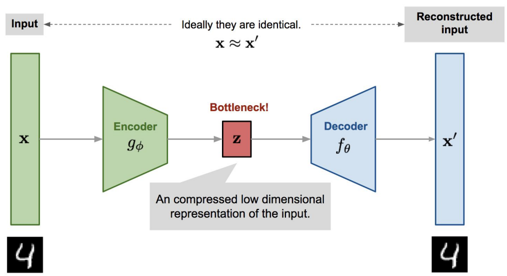

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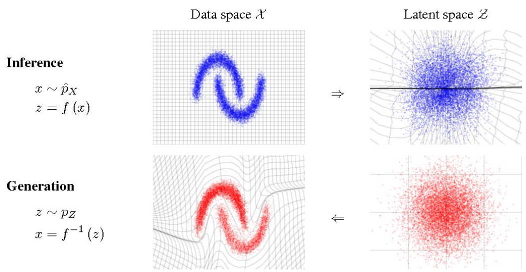
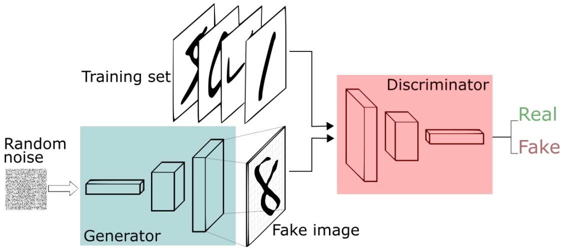
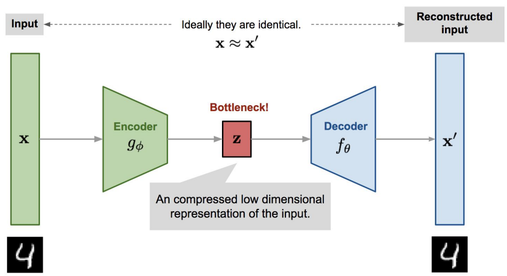
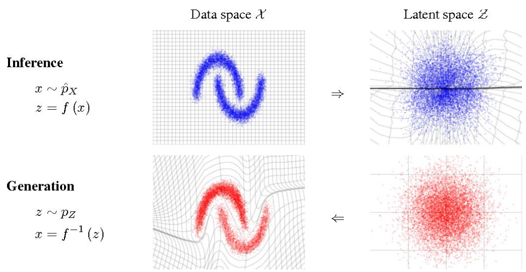


Flows

Generative modeling







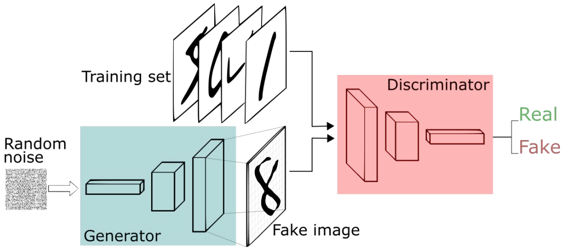
GANs

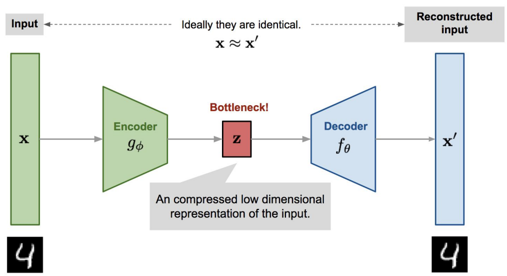
VAEs

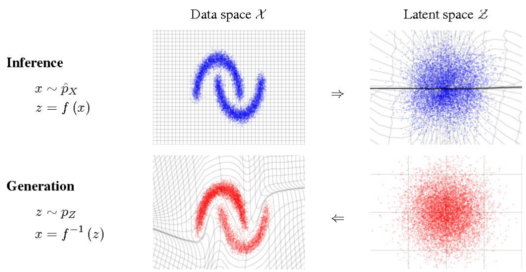
Flows

...

Generative modeling



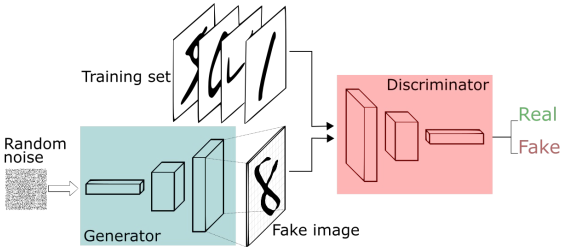


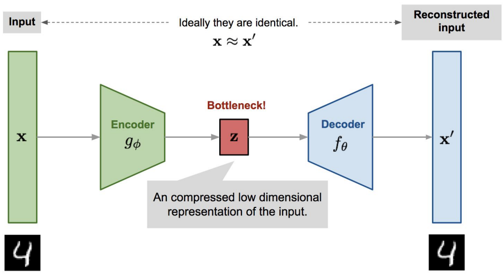


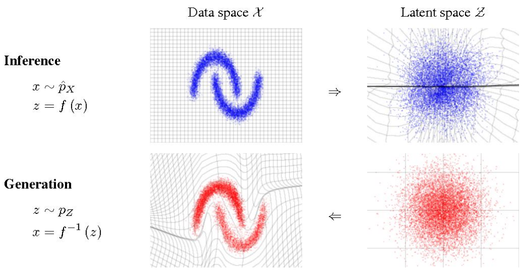
GANs | VAEs | Flows | ...

implicit (GANs) | explicit (VAEs, Flows)

Generative modeling







GANs VAEs Flows ...

implicitly explicitly

"learn" p(x)

“New” Idea:
Generative Modeling by Estimating Gradients of the Data Distribution

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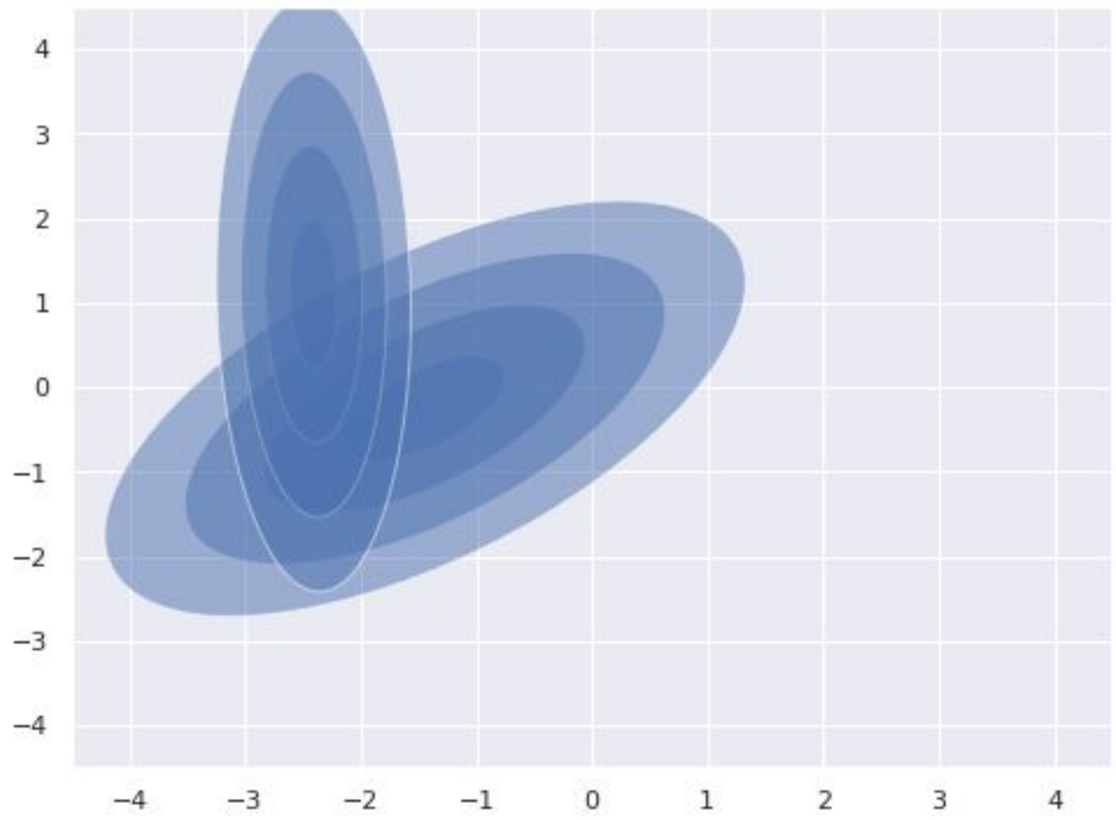
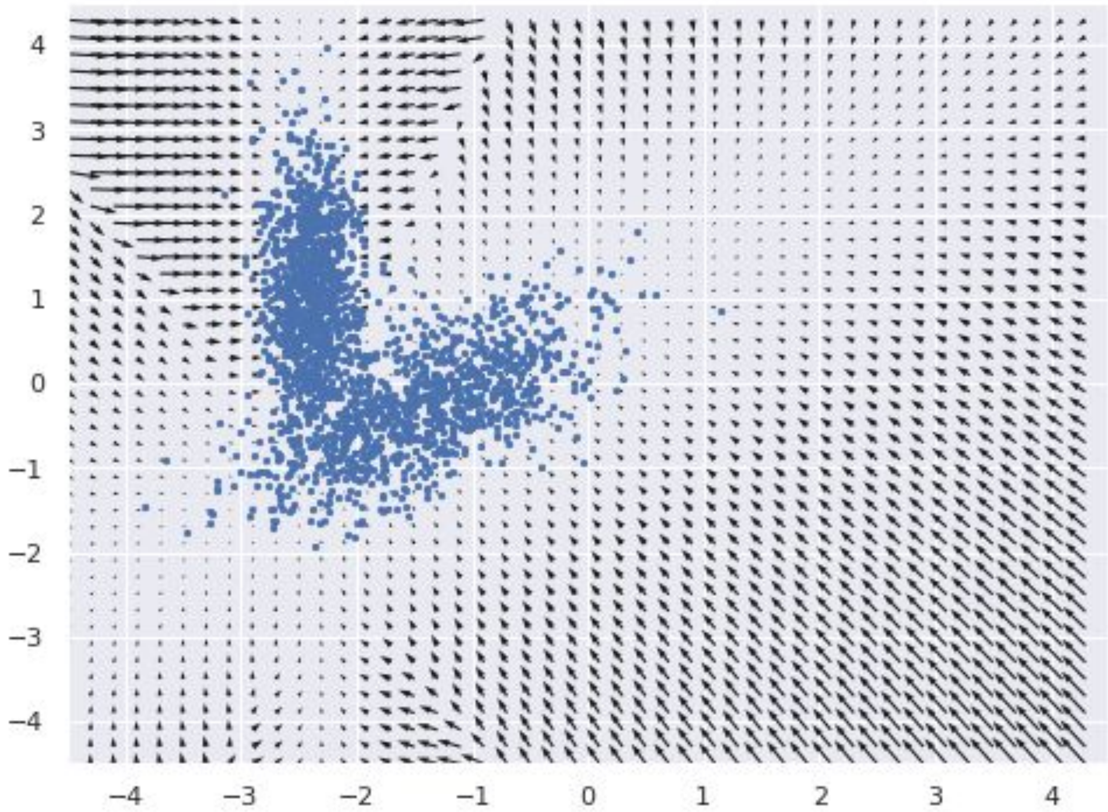


Instead of learning the data distribution directly....

“New” Idea:
Generative Modeling by Estimating Gradients of the Data Distribution



...we learn the gradients of the data distribution

“New” Idea:
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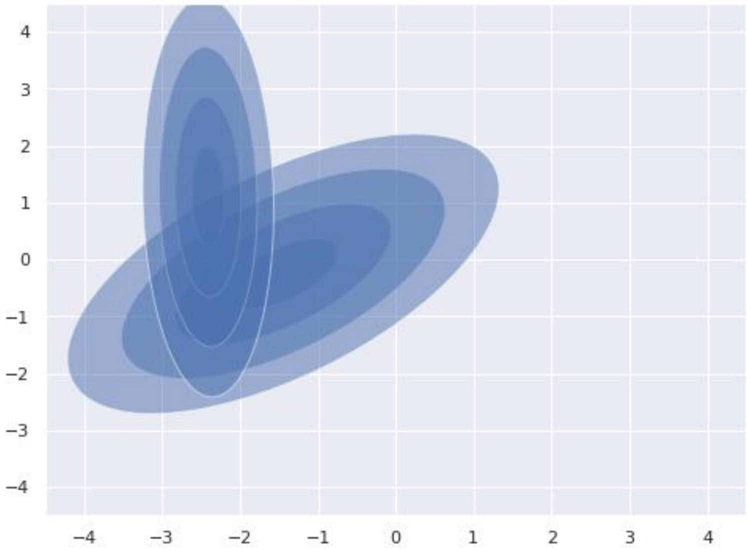

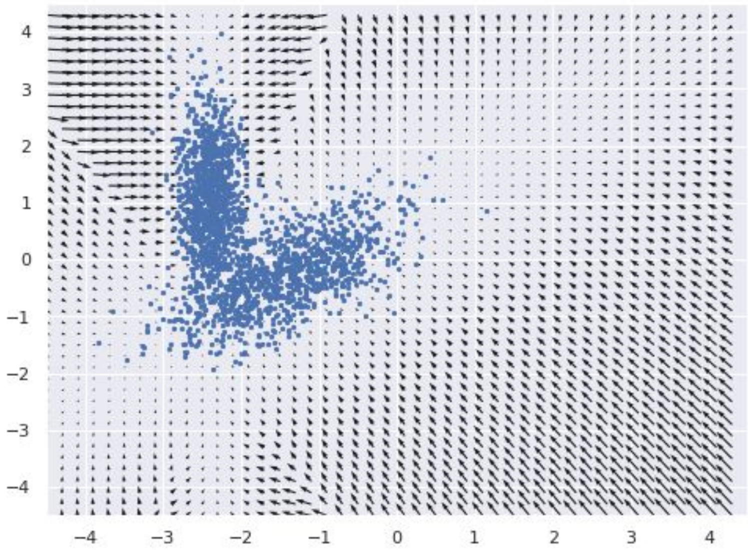

Score matching

[1] A. Hyvärinen. Estimation of non-normalized statistical models by score matching. Journal of Machine Learning Research, 6(Apr):695–709, 2005.

Score matching

$\rightarrow \nabla_{\mathbf{x}} \log p(\mathbf{x})$ i.e. the Gradient of the Data Distribution a.k.a *score*

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equivalent up to a constant to:

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$\rightarrow$ So what's new ? 🤔

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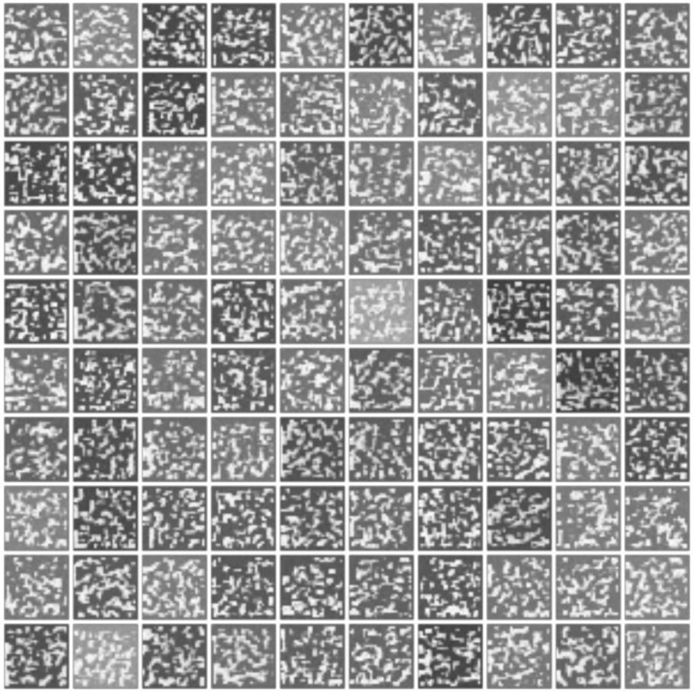

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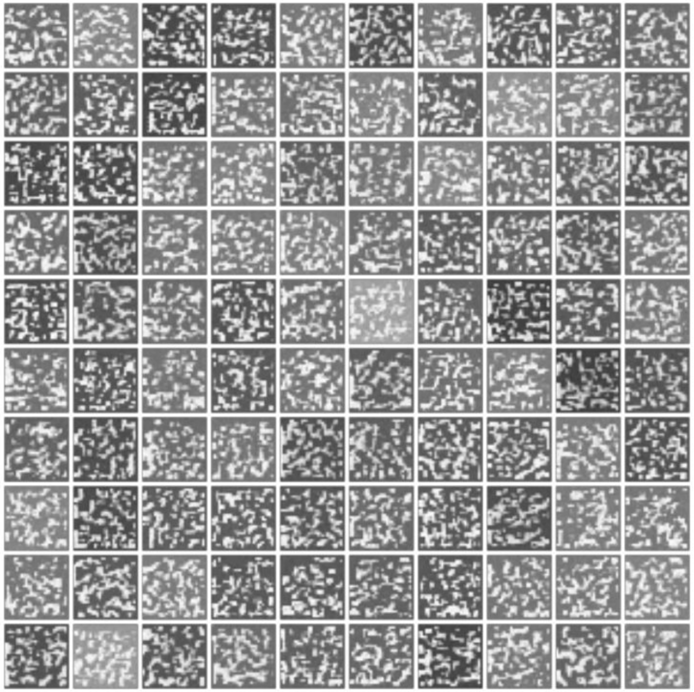

Spoiler: Improved Results

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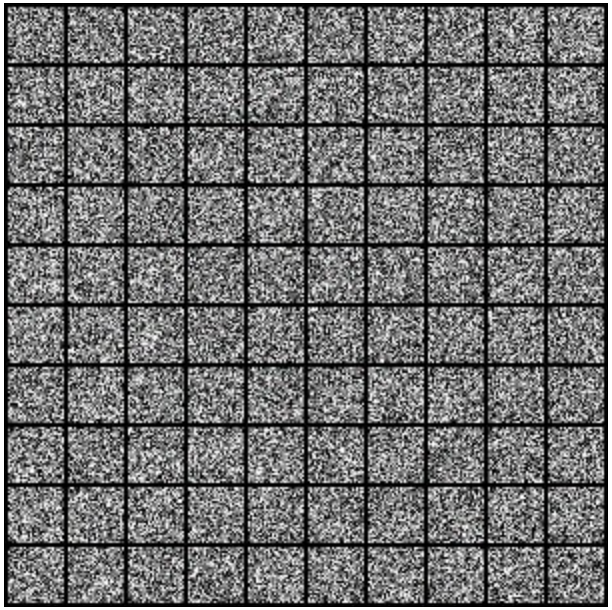

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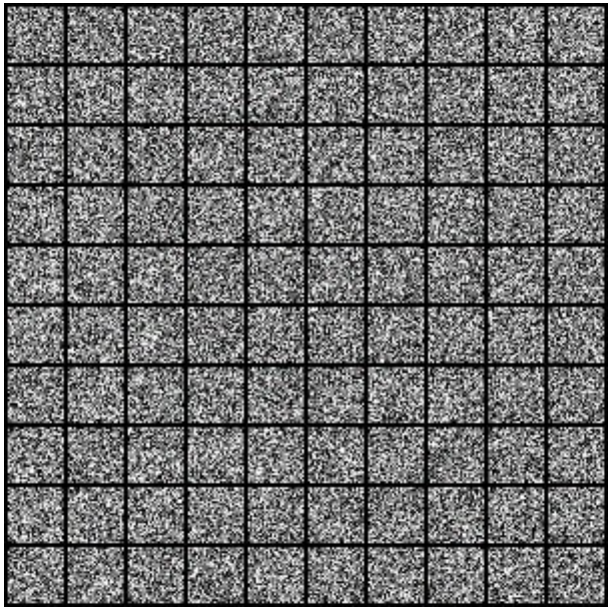

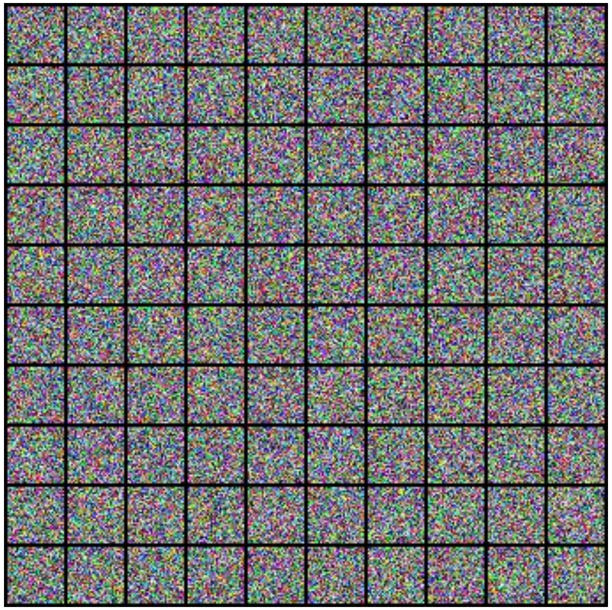

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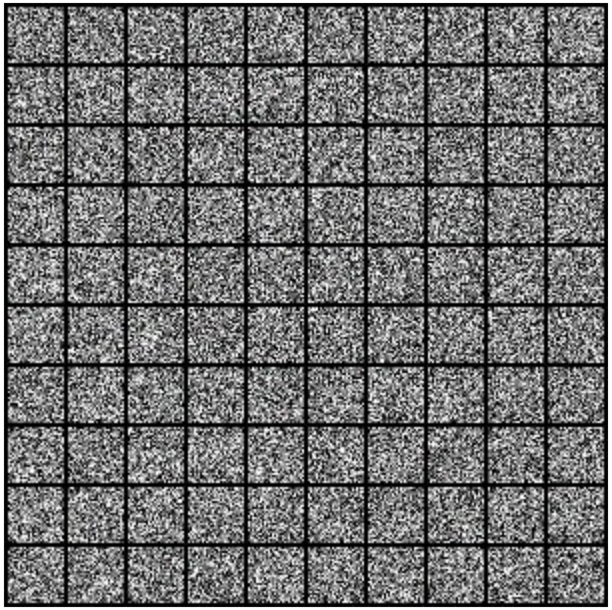

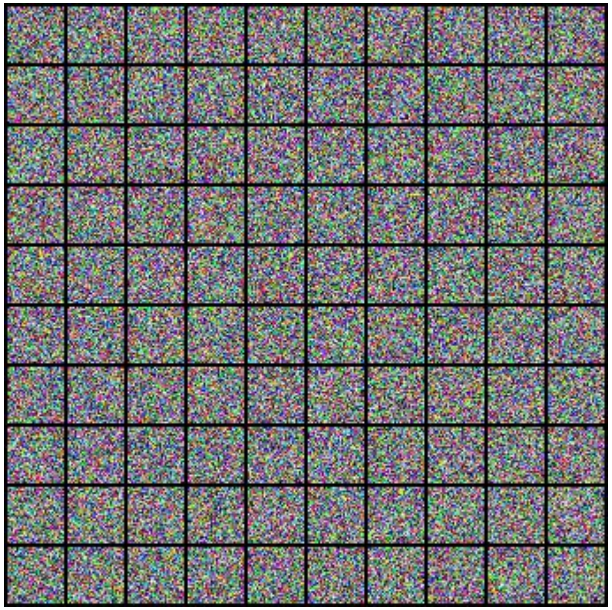

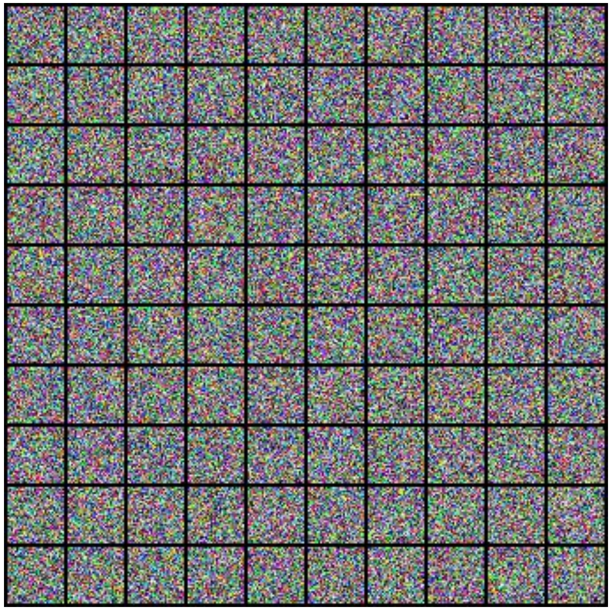

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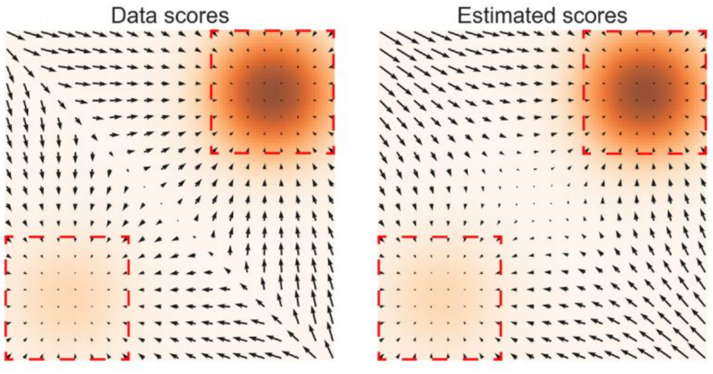

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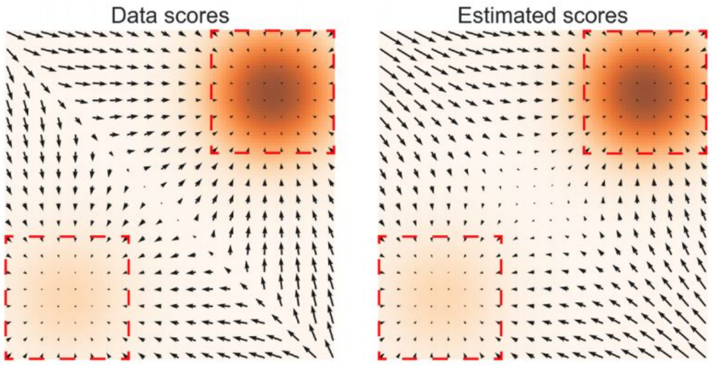

→ Solution add noise at different magnitudes

(large noise: filling low density regions, small noise: fine-adjustments in high density regions)

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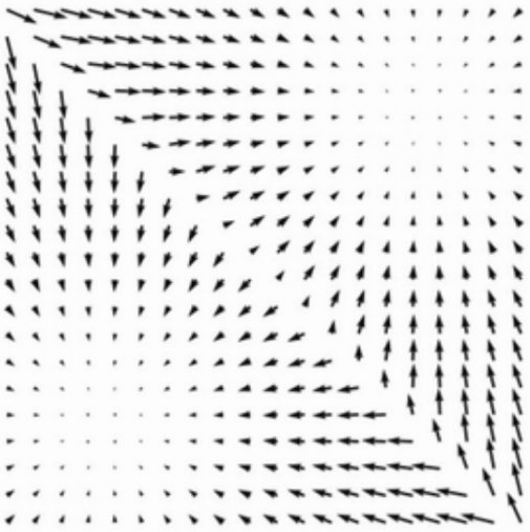

Scores

$s_\theta(\mathbf{x})$

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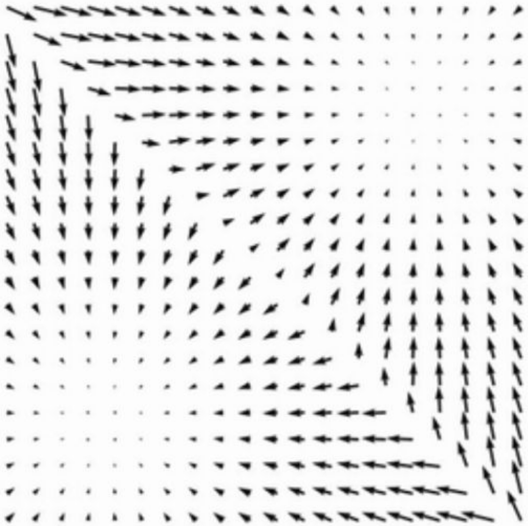

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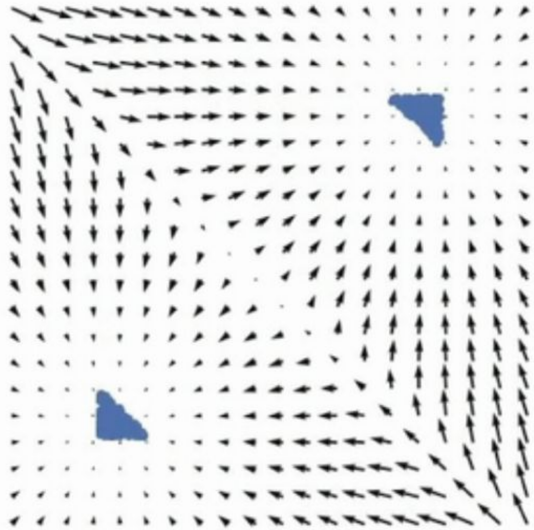

Follow the scores

$$\tilde{\mathbf{x}}_{t+1} \leftarrow \tilde{\mathbf{x}}_t + \frac{\epsilon}{2} s_\theta(\tilde{\mathbf{x}}_t)$$

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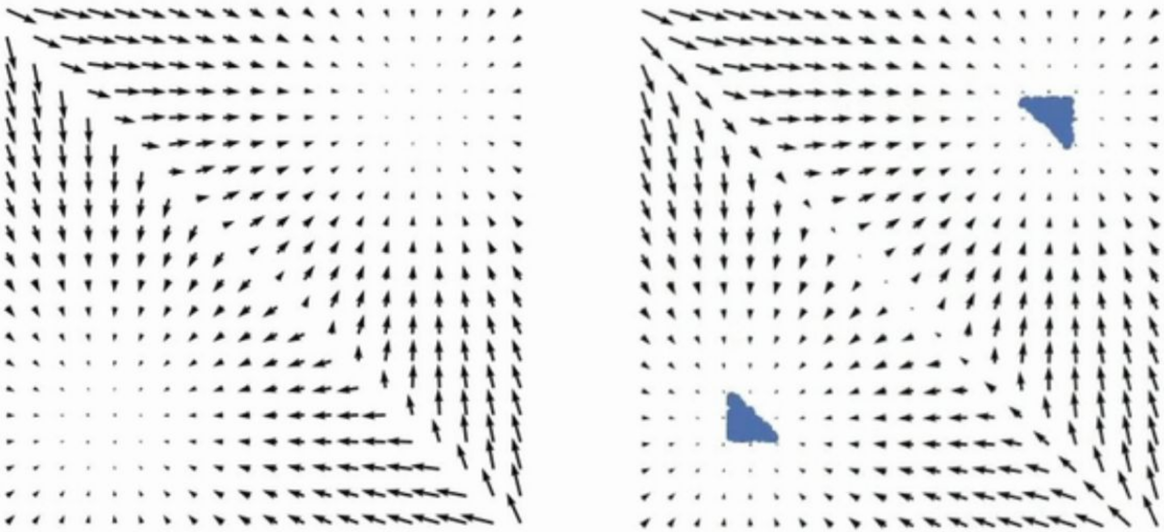

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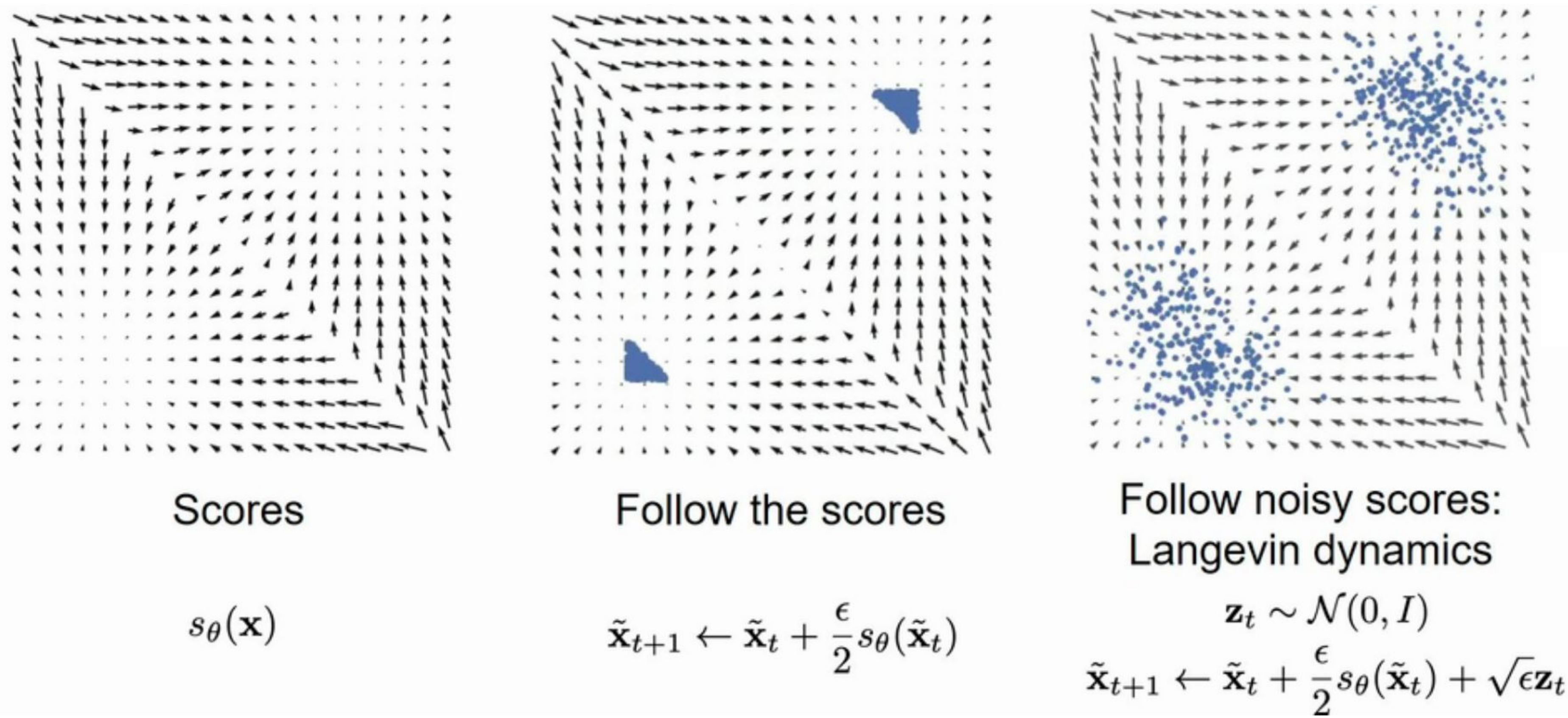

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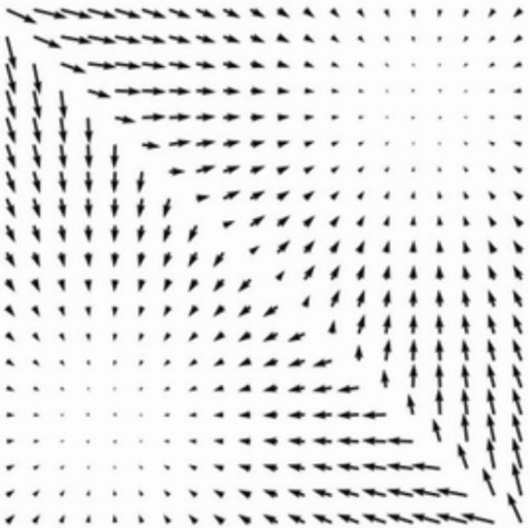

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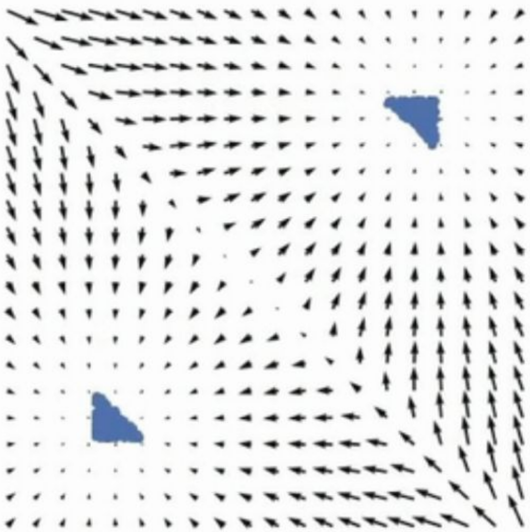

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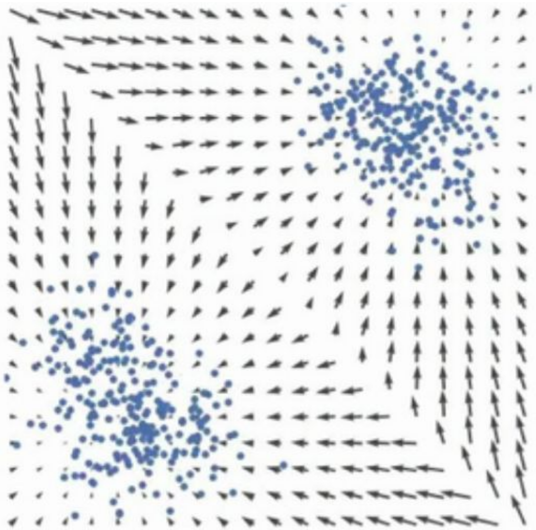

Follow noisy scores:
Langevin dynamics

$$\mathbf{z}_t \sim \mathcal{N}(0, I)$$

$$\tilde{\mathbf{x}}_{t+1} \leftarrow \tilde{\mathbf{x}}_t + \frac{\epsilon}{2} s_\theta(\tilde{\mathbf{x}}_t) + \sqrt{\epsilon}\mathbf{z}_t$$

Approach

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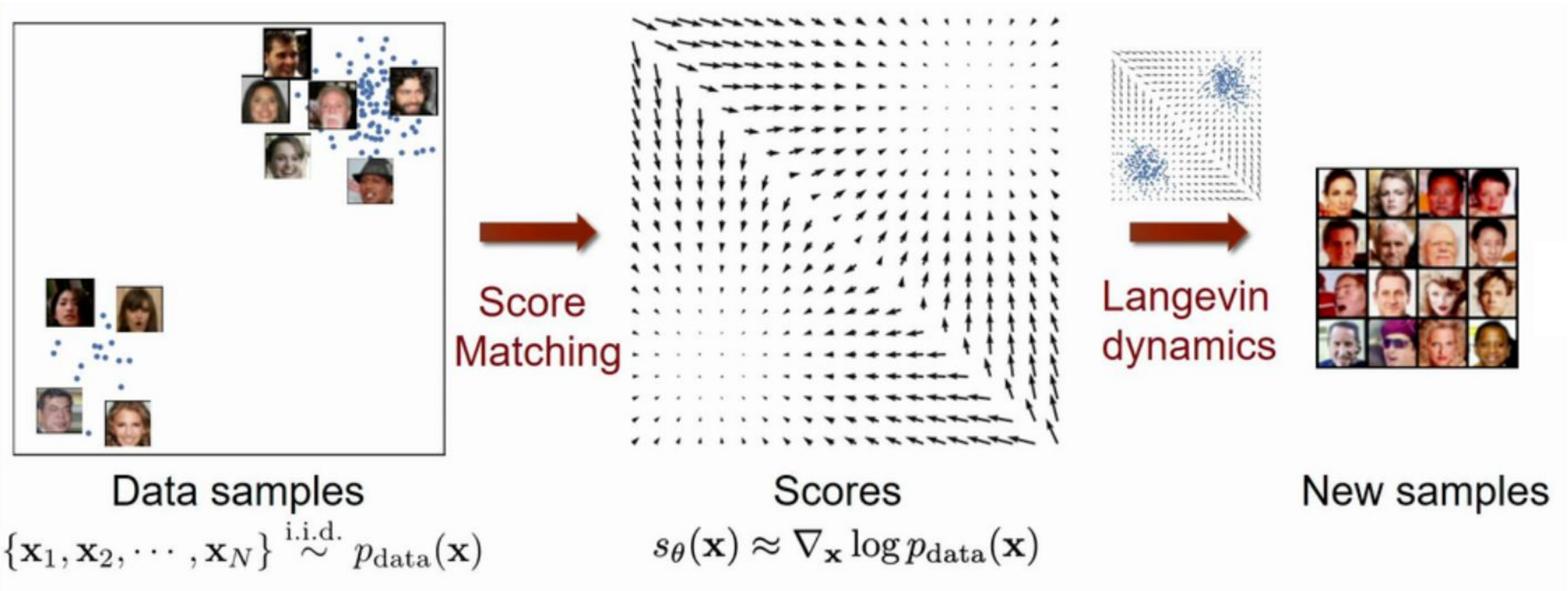

Score Matching
Langevin dynamics
Data samples
$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p_{\text{data}}(\mathbf{x})$
Scores
$s_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$
New samples

Results

Results: Qualitative

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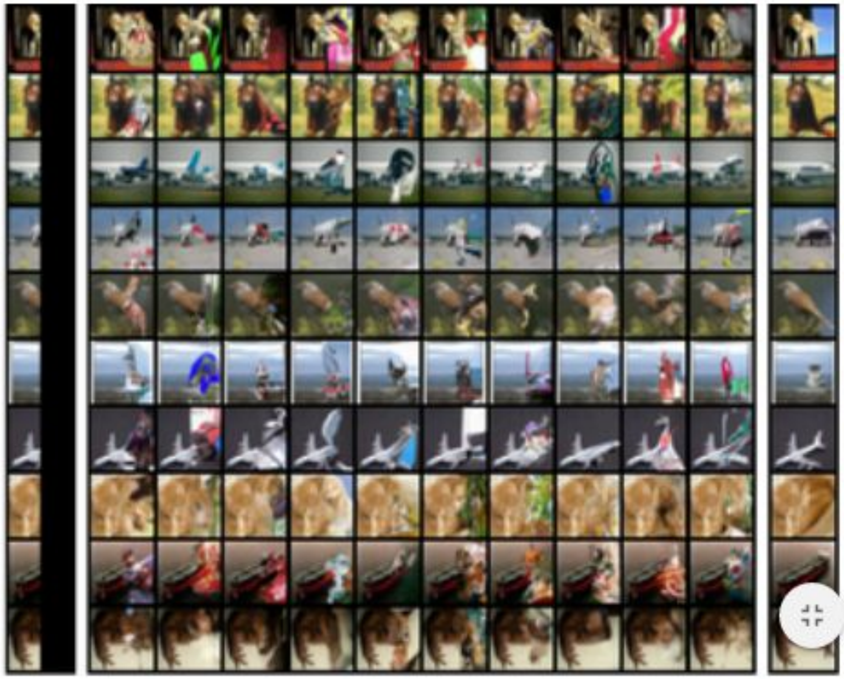

Results: Quantitative

Model	Inception ⇧	FID ⇩
CIFAR-10 Unconditional		
PixelCNN [59]	4.60	65.93
PixelIQN [42]	5.29	49.46
EBM [12]	6.02	40.58
WGAN-GP [18]	$7.86 \pm .07$	36.4
MoLM [45]	$7.90 \pm .10$	**18.9**
SNGAN [36]	$8.22 \pm .05$	21.7
ProgressiveGAN [25]	$8.80 \pm .05$	-
NCSN (Ours)	$\mathbf{8.87} \pm .12$	25.32
CIFAR-10 Conditional		
EBM [12]	8.30	37.9
SNGAN [36]	$8.60 \pm .08$	25.5
BigGAN [6]	**9.22**	**14.73**

Results: Reproducible

→ NeurIPS 2019 - Reproducibility Challenge[2]

[2] A. Matosevic. Reproducibility Challenge – Generative Modeling by Estimating Gradients of the Data Distribution, NeurIPS 2019 Reproducibility Challenge Blind Report, https://openreview.net/forum?id=SkxCSTqG6H

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The End