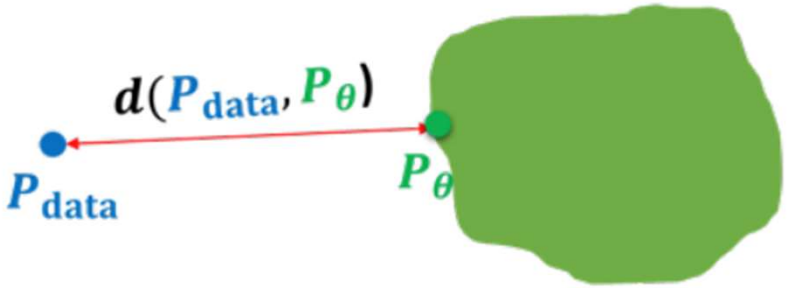
Score-Based Models

LECTURE 14

CS236: Deep Generative Models

Summary

$\mathbf{x}_i \sim P_{\text{data}}$
$i = 1, 2, \ldots, n$



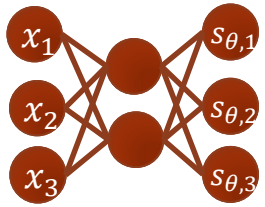
$\theta \in M$

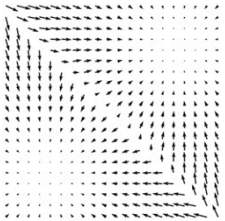
Model family

Score-based models

- A model that represents the score function

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





- **Score estimation:** training the score-based model from datapoints
- Score matching

$$\frac{1}{2}E_{\mathbf{x}\sim p_{\text{data}}}[\|\nabla_{\mathbf{x}}\log p_{\text{data}}(\mathbf{x}) - \boldsymbol{s}_\theta(\mathbf{x})\|_2^2]$$
$$=\frac{1}{2}E_{\mathbf{x}\sim p_{\text{data}}}\left[\frac{1}{2}\|\boldsymbol{s}_\theta(\mathbf{x})\|_2^2 + \text{tr}(\nabla_{\mathbf{x}}\boldsymbol{s}_\theta(\mathbf{x}))\right] + \text{const.}$$

- Not scalable for deep score-based models and high dimensional data

Denoising score matching

$\mathbf{x} \sim p_{\text{data}}(\mathbf{x})$

Data distribution

$q_\sigma(\tilde{\mathbf{x}} \mid \mathbf{x})$

Perturbation distribution/kernel

$\tilde{\mathbf{x}} \sim q_\sigma(\tilde{\mathbf{x}})$

Noise-perturbed data distribution

$$\frac{1}{2} E_{\tilde{\mathbf{x}} \sim p_{\text{data}}} [\| \boldsymbol{s}_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}}) \|_2^2]$$

$$= \frac{1}{2} E_{\mathbf{x} \sim p_{\text{data}}(\mathbf{x}), \tilde{\mathbf{x}} \sim q_\sigma(\tilde{\mathbf{x}} \mid \mathbf{x})} [\| \boldsymbol{s}_\theta(\tilde{\mathbf{x}}) - \nabla_{\tilde{\mathbf{x}}} \log q_\sigma(\tilde{\mathbf{x}} \mid \mathbf{x}) \|_2^2] + \text{const.}$$

$$= \frac{1}{2} E_{\mathbf{x} \sim p_{\text{data}}, \mathbf{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})} \left[\left\| \boldsymbol{s}_\theta(\mathbf{x} + \sigma \mathbf{z}) + \frac{\mathbf{z}}{\sigma} \right\|_2^2 \right] + \text{const.}$$

- **Pros:**
  - Much more scalable than score matching
  - Reduces score estimation to a denoising task
- **Con:** estimates score of noise-perturbed data

$$\boldsymbol{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log q_\sigma(\mathbf{x}) \neq \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$$

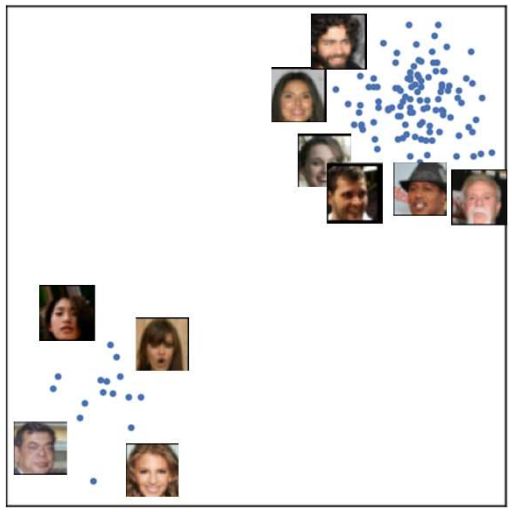
Sliced score matching

$$\frac{1}{2} E_{\mathbf{v}\sim p_{\mathbf{v}}} E_{\mathbf{x}\sim p_{\text{data}}} [(\mathbf{v}^\intercal \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - \mathbf{v}^\intercal \boldsymbol{s}_\theta(\mathbf{x}))^2]$$

$$= E_{\mathbf{v}\sim p_{\mathbf{v}}, \mathbf{x}\sim p_{\text{data}}} \left[\mathbf{v}^\intercal \nabla_{\mathbf{x}} \boldsymbol{s}_\theta(\mathbf{x}) \mathbf{v} + \frac{1}{2} (\mathbf{v}^\intercal \boldsymbol{s}_\theta(\mathbf{x}))^2 \right] + \text{const.}$$

- Projection distribution $p_{\mathbf{v}}$ can be Gaussian or Rademacher
- **Pros:**
  - Much more scalable than score matching;
  - Estimates the true data score.
- **Con**: Slower than denoising score matching.

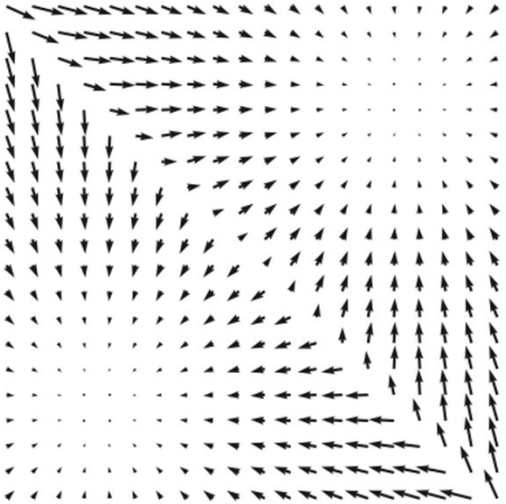
Score-based generative modeling



Data samples

$$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\} \sim p_{\text{data}}(\mathbf{x})$$

score matching



Scores

$$\boldsymbol{s}_\theta(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$$

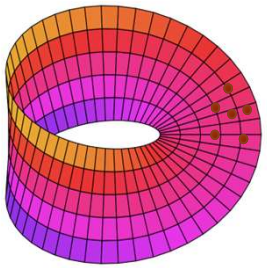
Langevin dynamics

New samples

Pitfalls

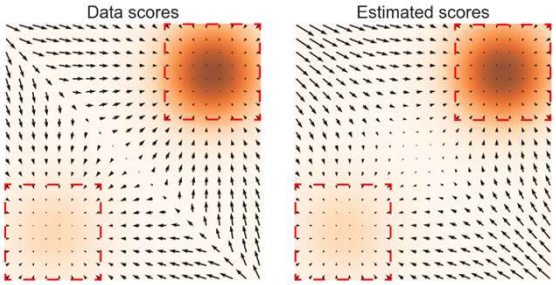
- Manifold hypothesis. Data score is undefined.

$$\times \nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x})$$

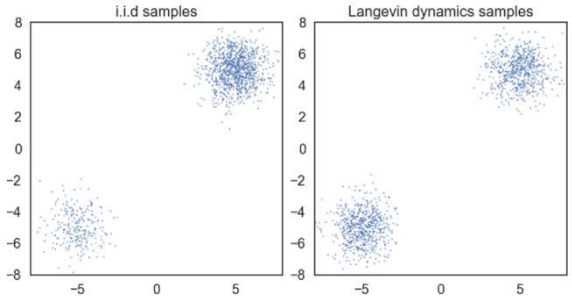


Data points

- Score matching fails in low data density regions

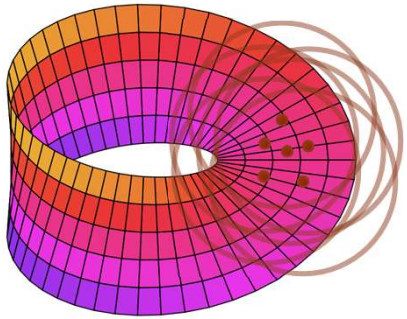


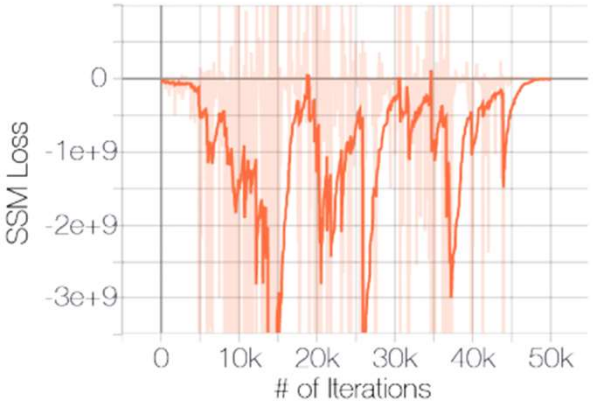
- Langevin dynamics converges very slowly



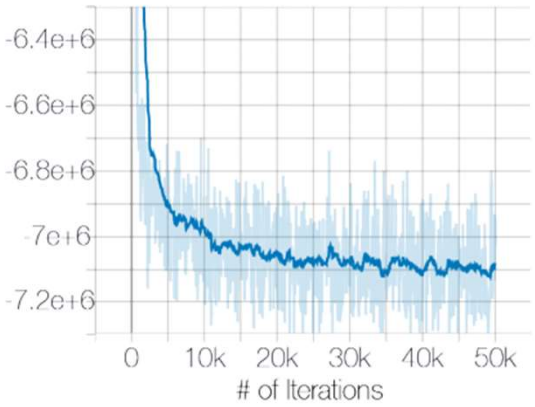
Gaussian perturbation

- The solution to all pitfalls: **Gaussian perturbation!**
- Manifold + noise
- Score matching on noisy data.





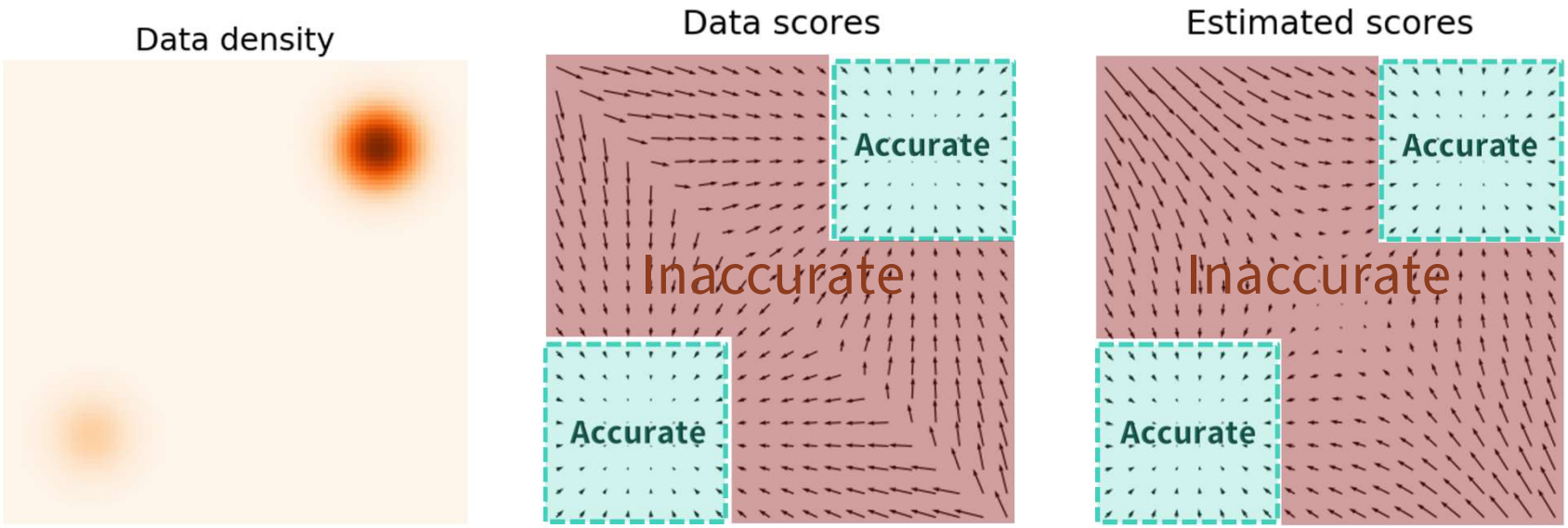
CIFAR-10



Noisy CIFAR-10

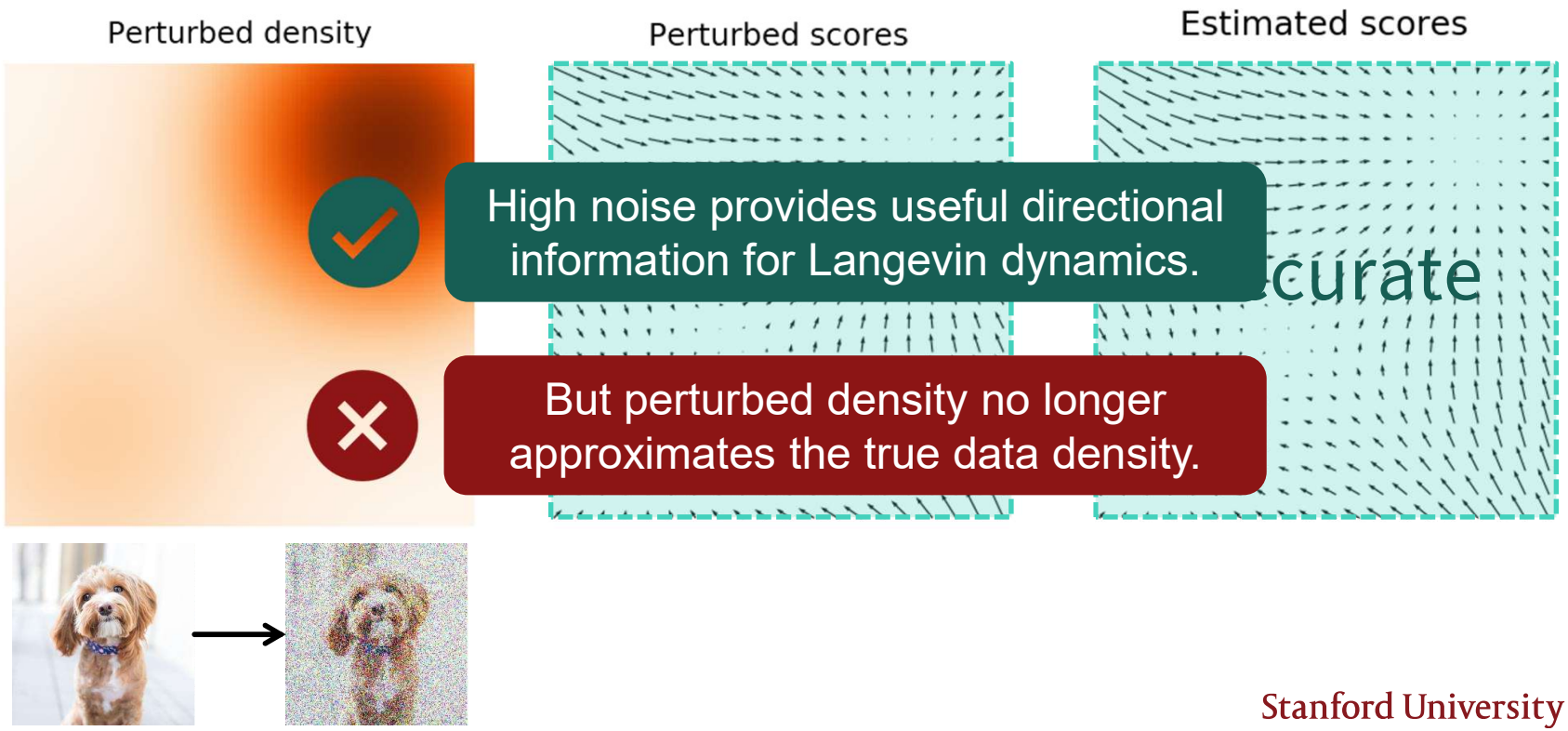
$$\mathcal{N}(0; 0.0001)$$

Challenge in low data density regions



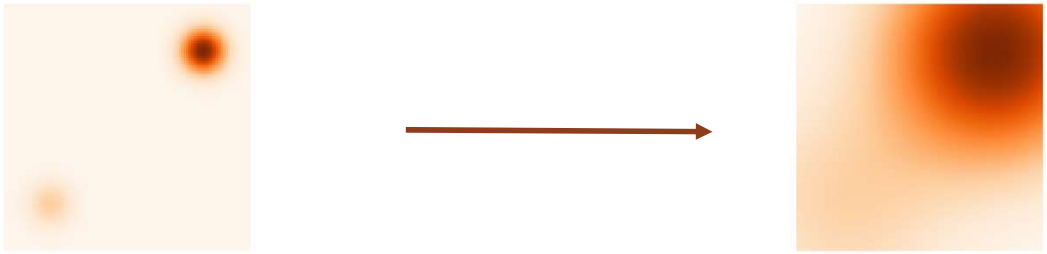
Song and Ermon. “Generative Modeling by Estimating Gradients of the Data Distribution.” NeurIPS 2019.

Improving score estimation by adding noise



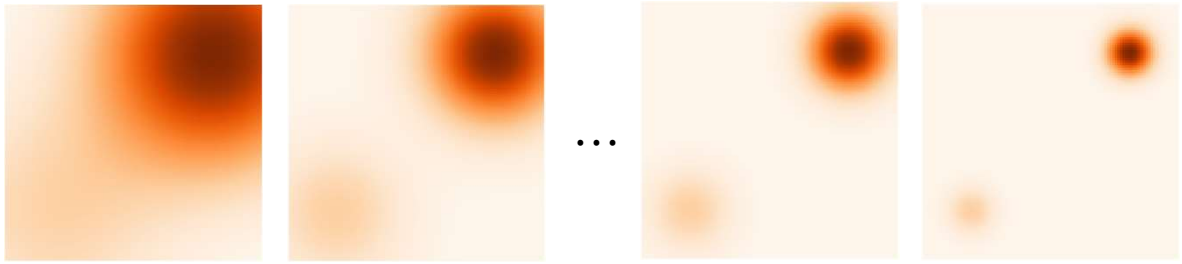
Multi-scale Noise Perturbation

- How much noise to add?

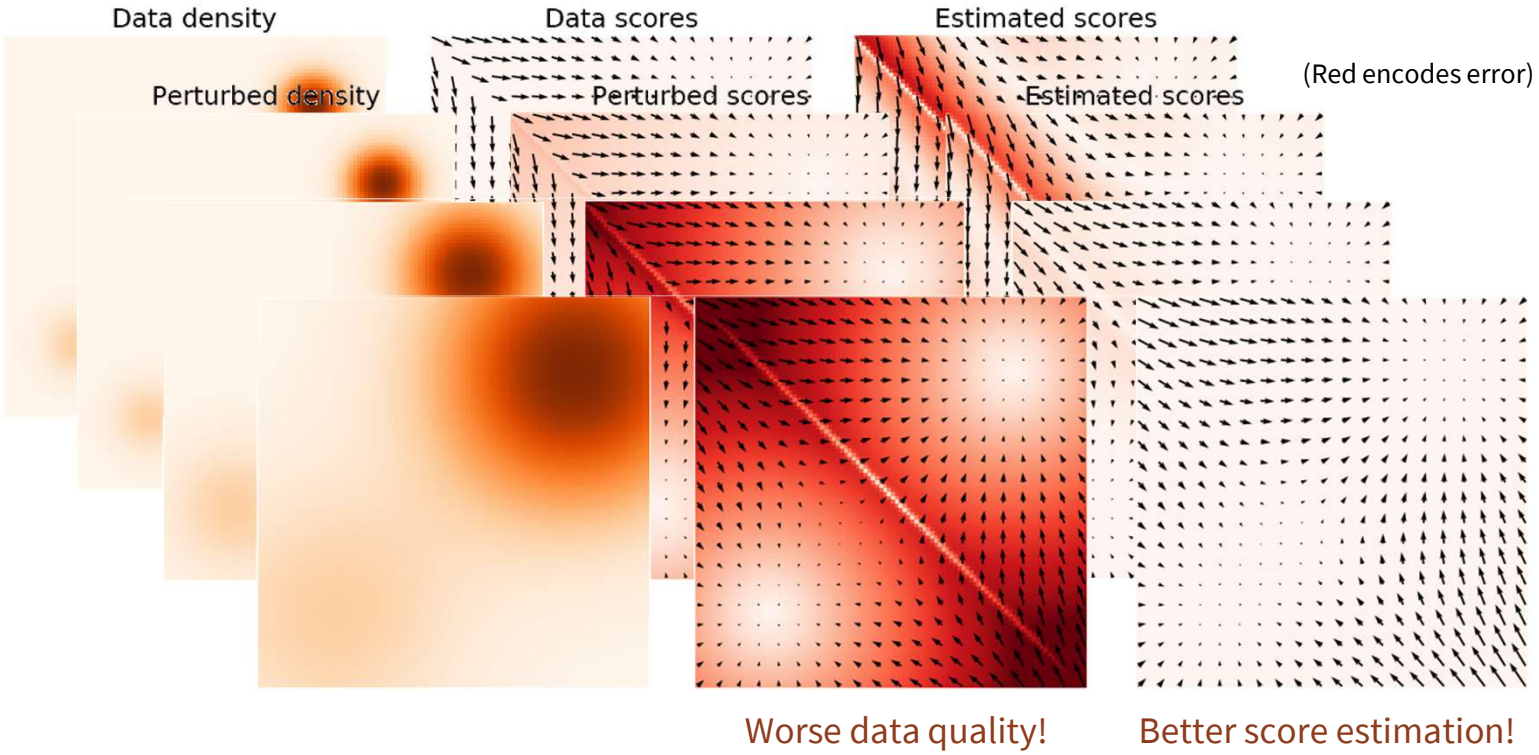


- Multi-scale noise perturbations.

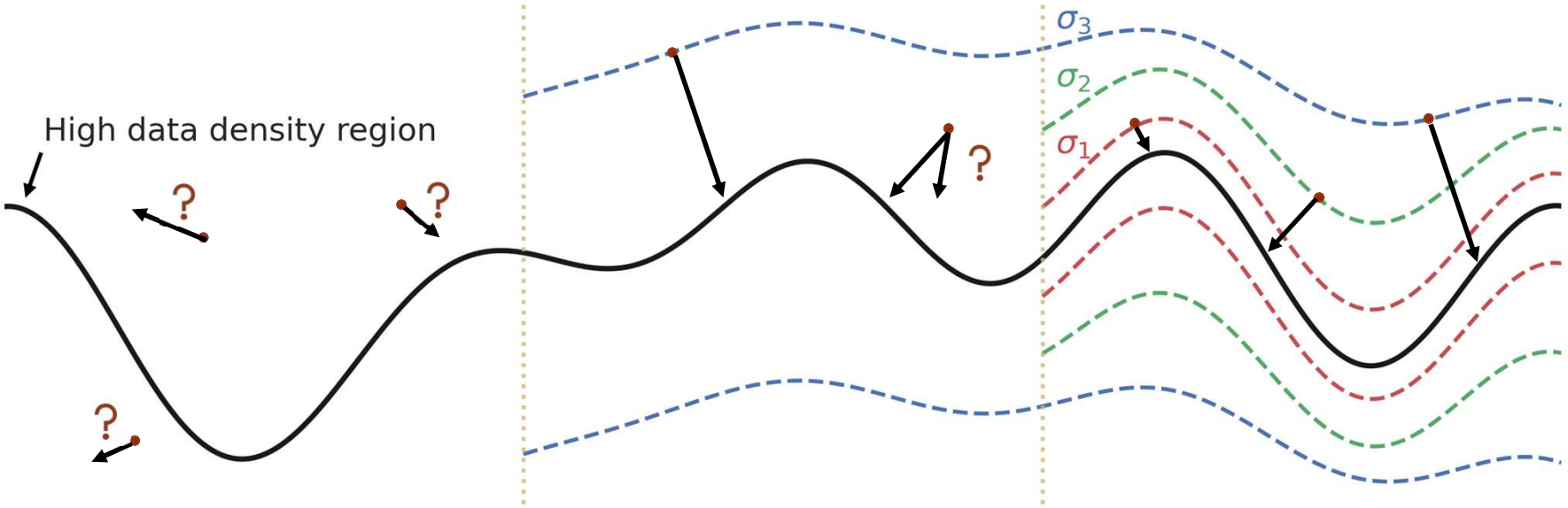
$$\sigma_1 > \sigma_2 > \cdots > \sigma_{L-1} > \sigma_L$$



Trading off Data Quality and Estimation Accuracy

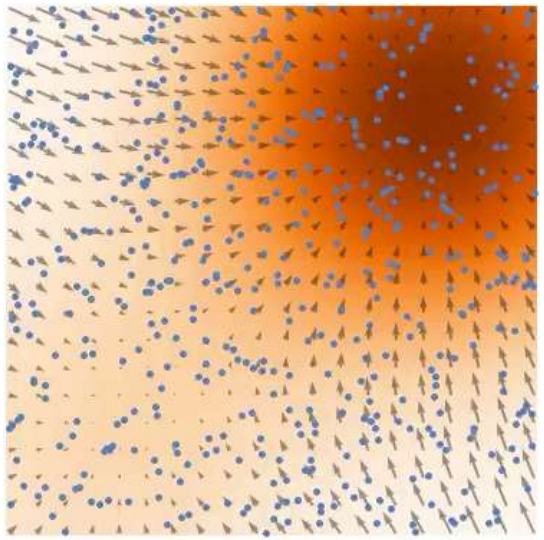


Using multiple noise scales

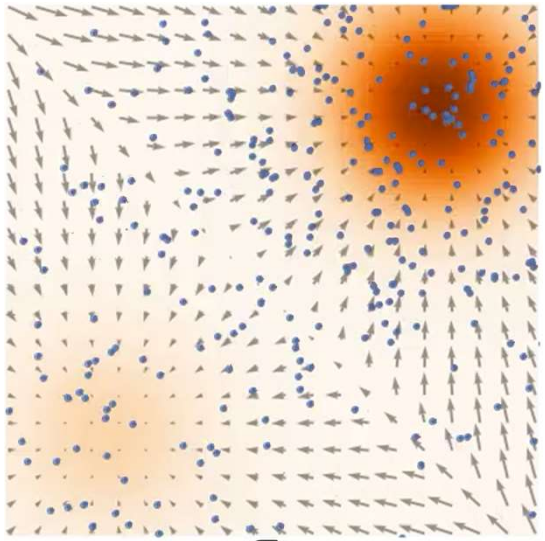


Annealed Langevin Dynamics: Joint Scores to Samples

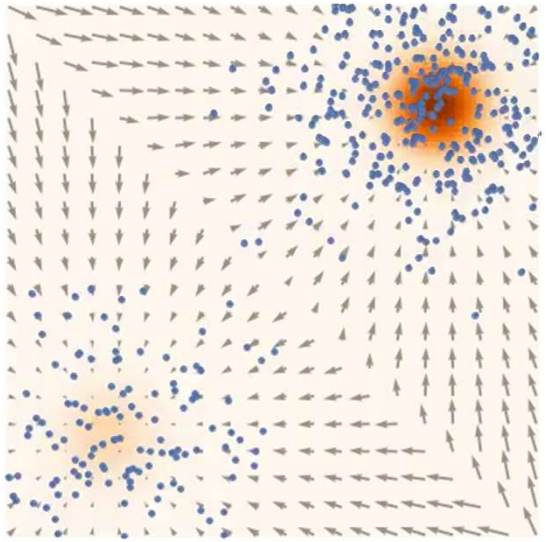
- Sample using $\sigma_1, \sigma_2, \cdots, \sigma_L$ sequentially with Langevin dynamics.
- Anneal down the noise level.
- Samples used as initialization for the next level.



σ_1

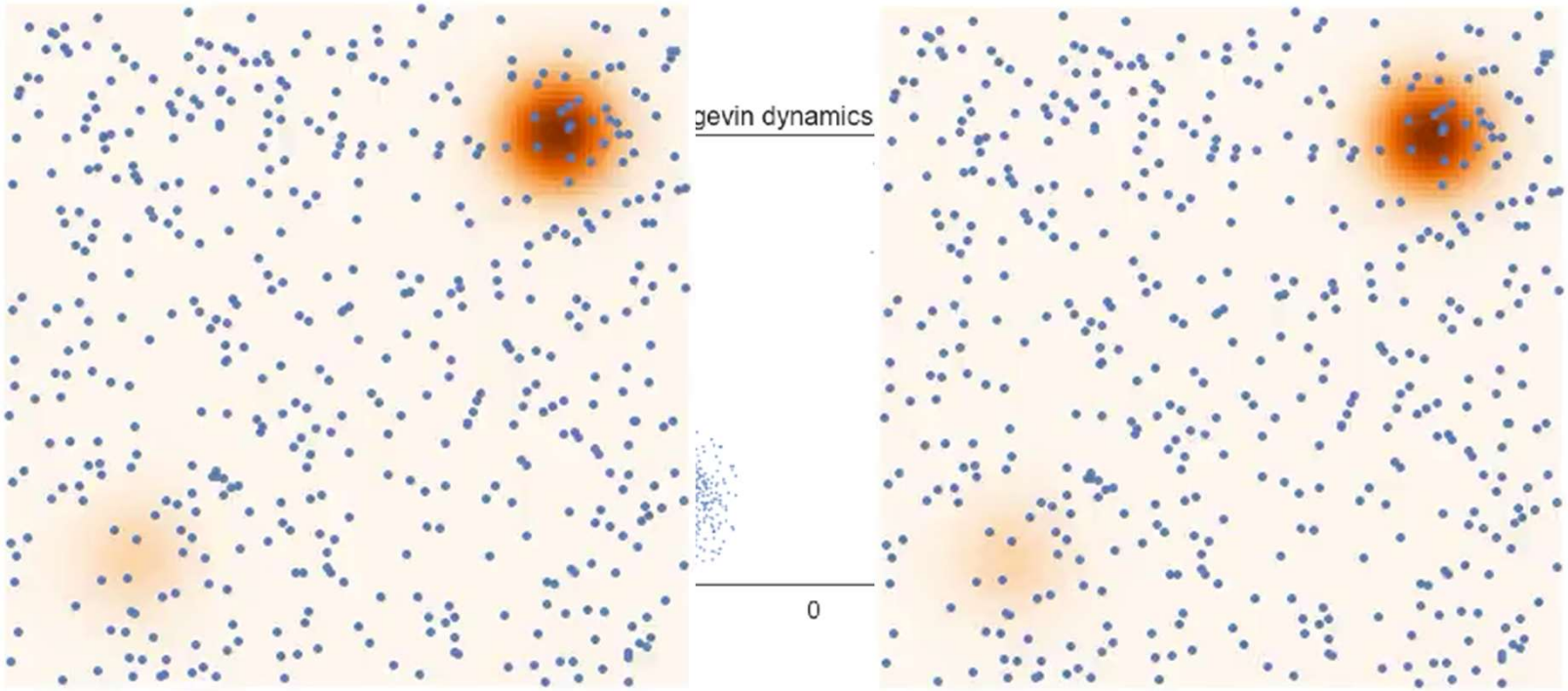


σ_2



σ_3

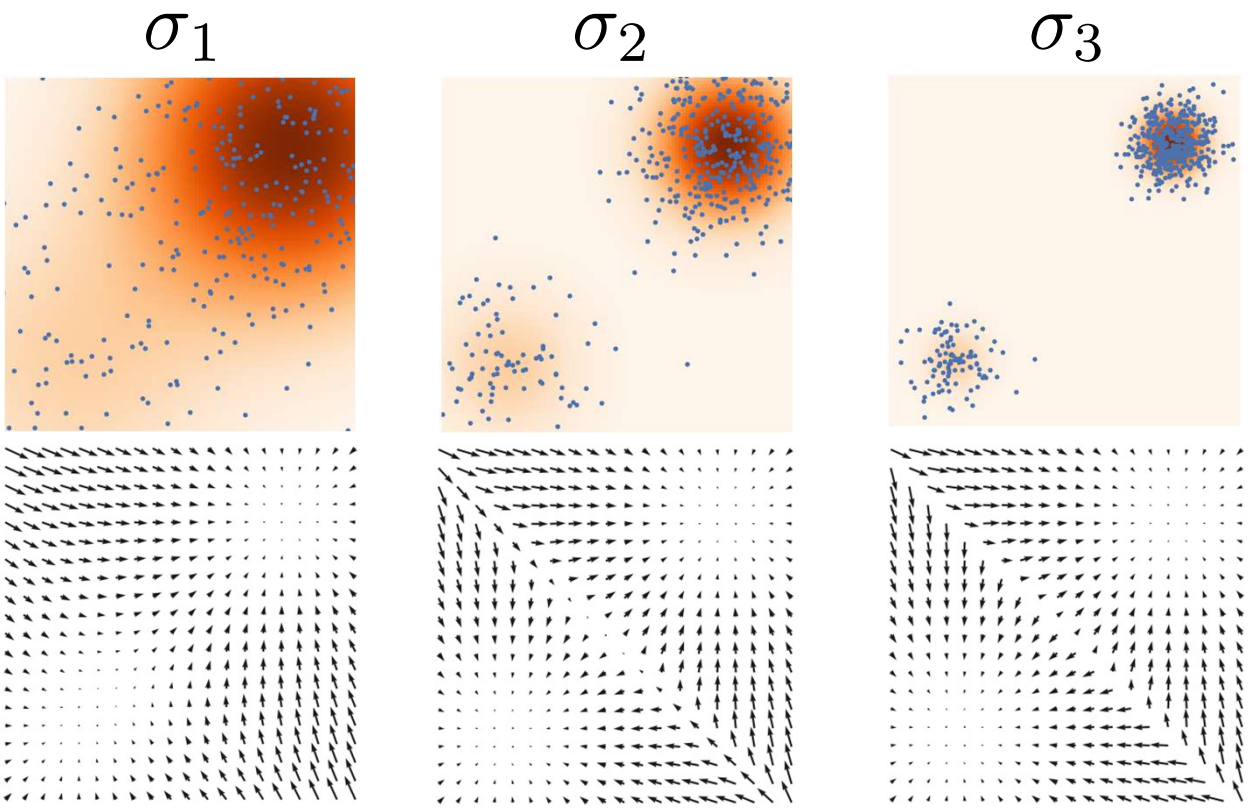
Comparison to the vanilla Langevin dynamics

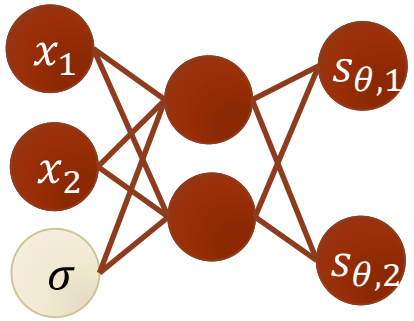


Langevin dynamics

Annealed Langevin dynamics

Joint Score Estimation via Noise Conditional Score Networks





Noise Conditional Score Network (NCSN)

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Training noise conditional score networks

- Which score matching loss?
  - Sliced score matching?
  - Denoising score matching?
- Denoising score matching is naturally suitable, since the goal is to estimate the score of perturbed data distributions.
- Weighted combination of denoising score matching losses

$$\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)E_{q_{\sigma_i}(\mathbf{x})}[\|\nabla_{\mathbf{x}}\log q_{\sigma_i}(\mathbf{x})-\boldsymbol{s}_\theta(\mathbf{x},\sigma_i)\|_2^2]$$

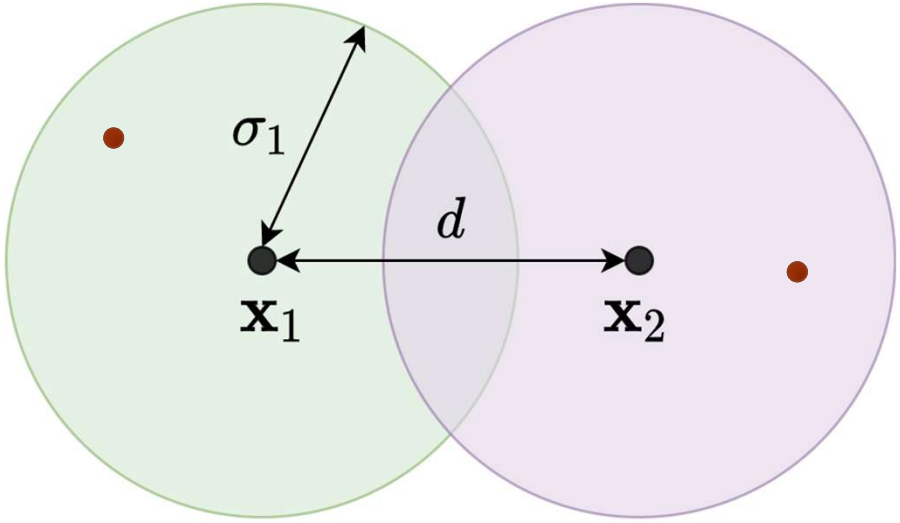
$$=\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}[\|\nabla_{\tilde{\mathbf{x}}}\log q_{\sigma_i}(\tilde{\mathbf{x}}\mid\mathbf{x})-\boldsymbol{s}_\theta(\tilde{\mathbf{x}},\sigma_i)\|_2^2]+\text{const.}$$

$$=\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\left\|\boldsymbol{s}_\theta(\mathbf{x}+\sigma_i\mathbf{z},\sigma_i)+\frac{\mathbf{z}}{\sigma_i}\right\|_2^2\right]+\text{const.}$$

Choosing noise scales

- Maximum noise scale

$$\sigma_1 \approx \text{maximum pairwise distance between datapoints}$$



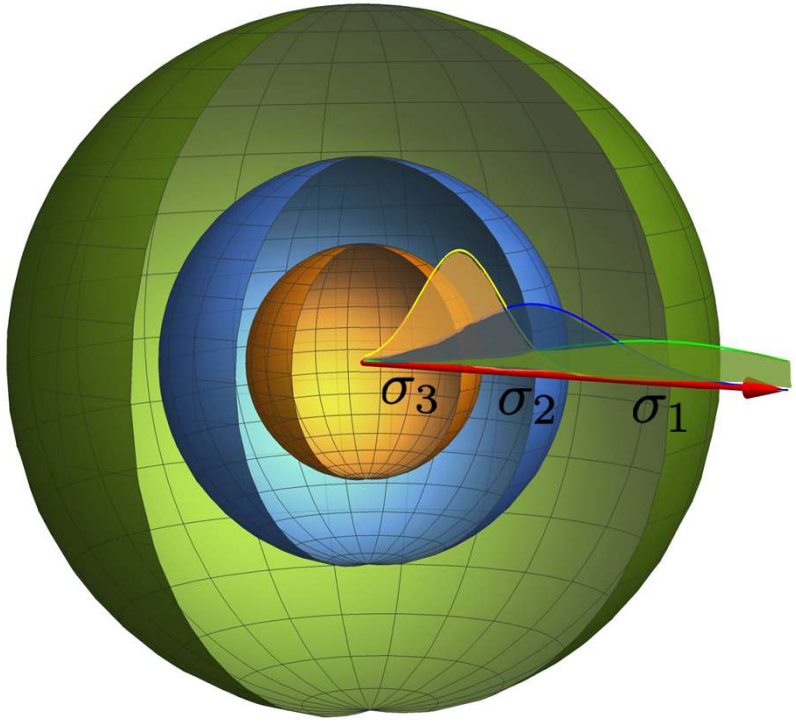
- Minimum noise scale: σ_L should be sufficiently small so that noise in final samples is negligible.

Choosing noise scales

- **Key intuition:** adjacent noise scales should have sufficient overlap to facilitate transitioning across noise scales in annealed Langevin dynamics.
- A geometric progression with sufficient length.

$$\sigma_1 > \sigma_2 > \sigma_3 > \cdots > \sigma_{L-1} > \sigma_L$$

$$\frac{\sigma_1}{\sigma_2} = \frac{\sigma_2}{\sigma_3} = \cdots = \frac{\sigma_{L-1}}{\sigma_L}$$



Choosing the weighting function

- Weighted combination of denoising score matching losses

$$\frac{1}{L}\sum_{i=1}^{L}\lambda(\sigma_i)E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\left\|\boldsymbol{s}_\theta(\mathbf{x}+\sigma_i\mathbf{z},\sigma_i)+\frac{\mathbf{z}}{\sigma_i}\right\|_2^2\right]$$

- How to choose the weighting function $\lambda : \mathbb{R}_{>0} \rightarrow \mathbb{R}_{>0}$?
- **Goal:** balancing different score matching losses in the sum → $\lambda(\sigma_i) = \sigma_i^2$

$$\begin{aligned}
&\frac{1}{L}\sum_{i=1}^{L}\sigma_i^2 E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\left\|\boldsymbol{s}_\theta(\mathbf{x}+\sigma_i\mathbf{z},\sigma_i)+\frac{\mathbf{z}}{\sigma_i}\right\|_2^2\right] \\
=&\frac{1}{L}\sum_{i=1}^{L}E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\left\|\sigma_i\boldsymbol{s}_\theta(\mathbf{x}+\sigma_i\mathbf{z},\sigma_i)+\mathbf{z}\right\|_2^2\right] \\
=&\frac{1}{L}\sum_{i=1}^{L}E_{\mathbf{x}\sim p_{\text{data}},\mathbf{z}\sim\mathcal{N}(\mathbf{0},\boldsymbol{I})}\left[\left\|\boldsymbol{\epsilon}_\theta(\mathbf{x}+\sigma_i\mathbf{z},\sigma_i)+\mathbf{z}\right\|_2^2\right] \qquad [\ \boldsymbol{\epsilon}_\theta(\cdot,\sigma_i) := \sigma_i\boldsymbol{s}_\theta(\cdot,\sigma_i)\ ]
\end{aligned}$$

Training noise conditional score networks

- Sample a mini-batch of datapoints $\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_n\} \sim p_{\text{data}}$
- Sample a mini-batch of noise scale indices

$$\{i_1, i_2, \cdots, i_n\} \sim \mathcal{U}\{1, 2, \cdots, L\}$$

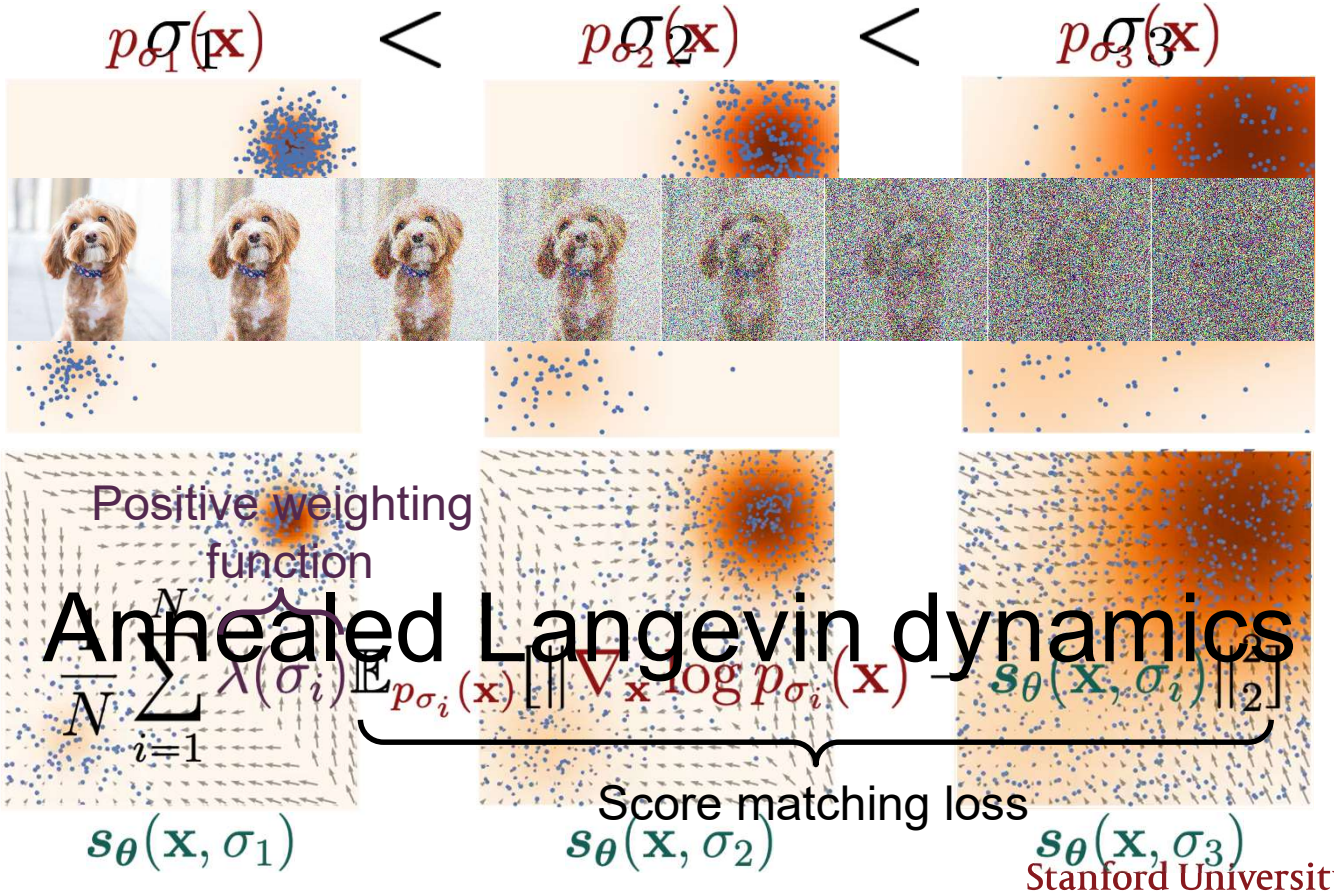
- Sample a mini-batch of Gaussian noise $\{\mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_n\} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I})$
- Estimate the weighted mixture of score matching losses

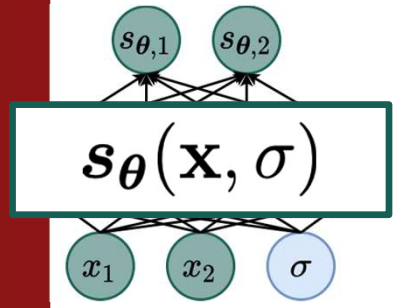
$$\frac{1}{n} \sum_{k=1}^{n} \left[\left\| \sigma_{i_k} \boldsymbol{s}_\theta(\mathbf{x}_k + \sigma_{i_k} \mathbf{z}_k, \sigma_{i_k}) + \mathbf{z}_k \right\|_2^2 \right]$$

- Stochastic gradient descent
- As efficient as training one single non-conditional score-based model

Using multiple noise levels

Data

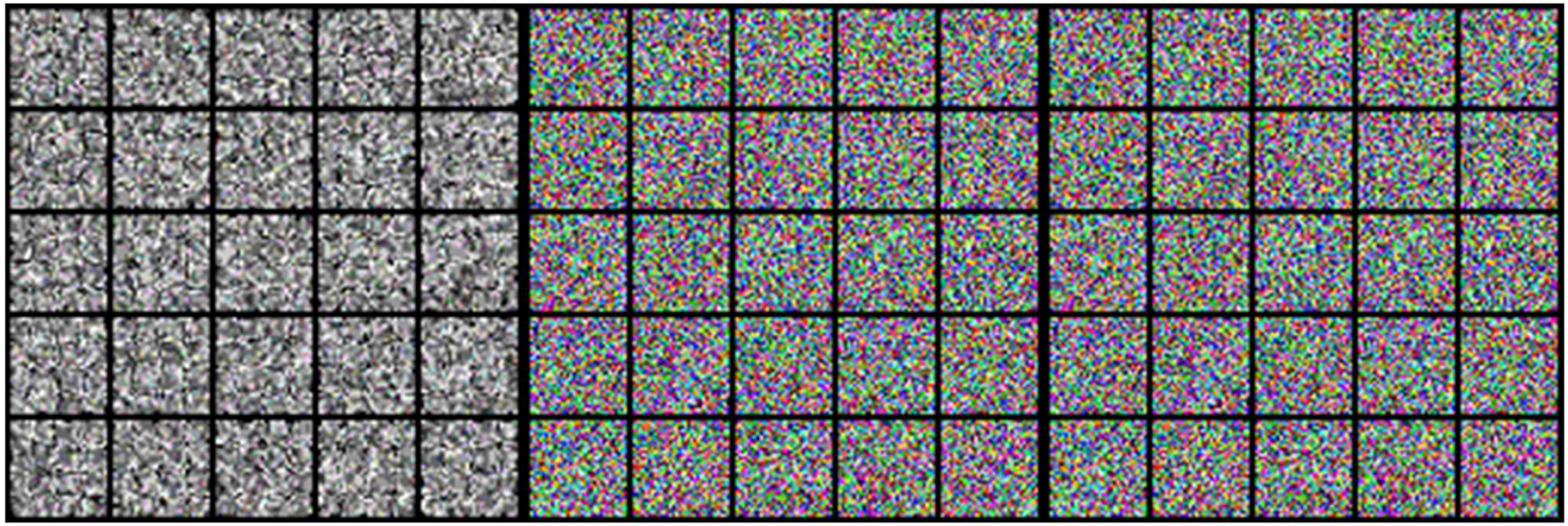




Noise Conditional Score Model

Annealed Langevin dynamics

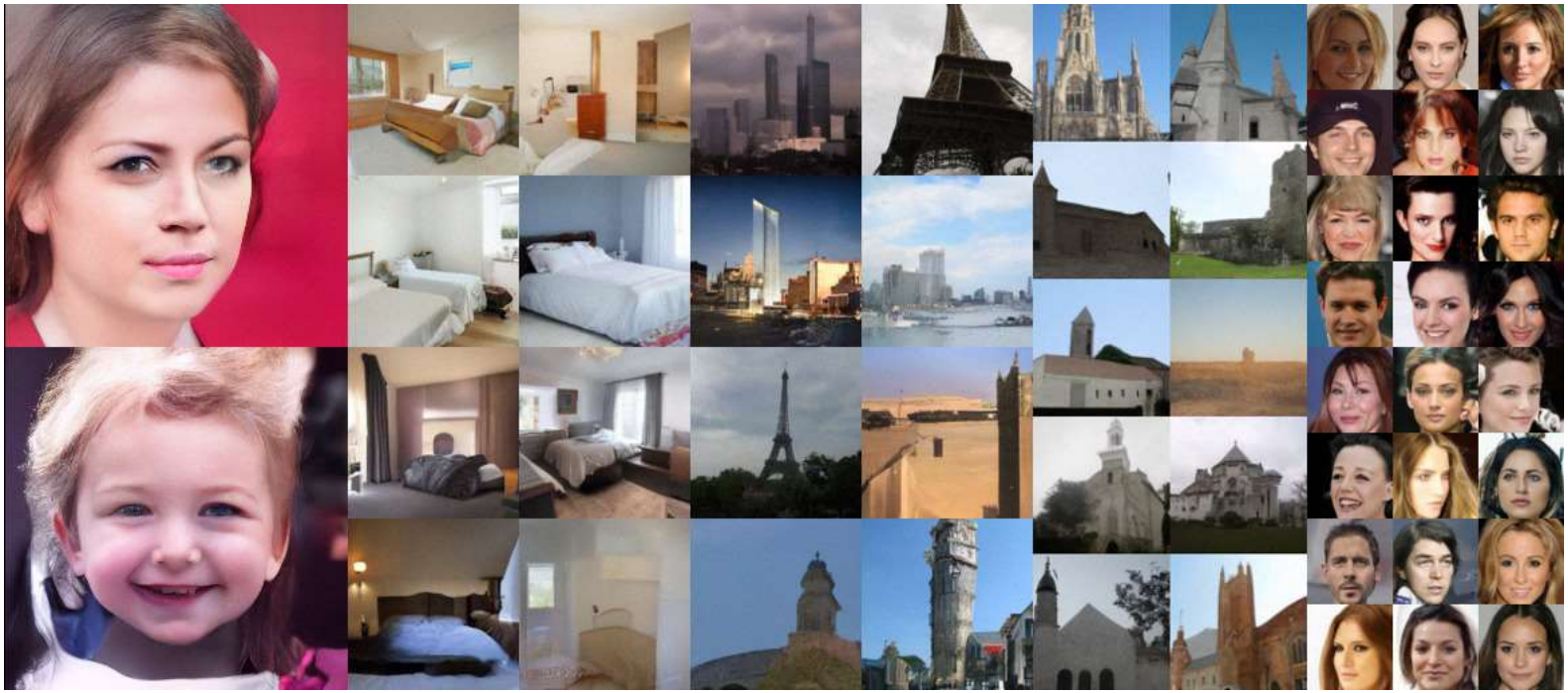
Experiments: Sampling



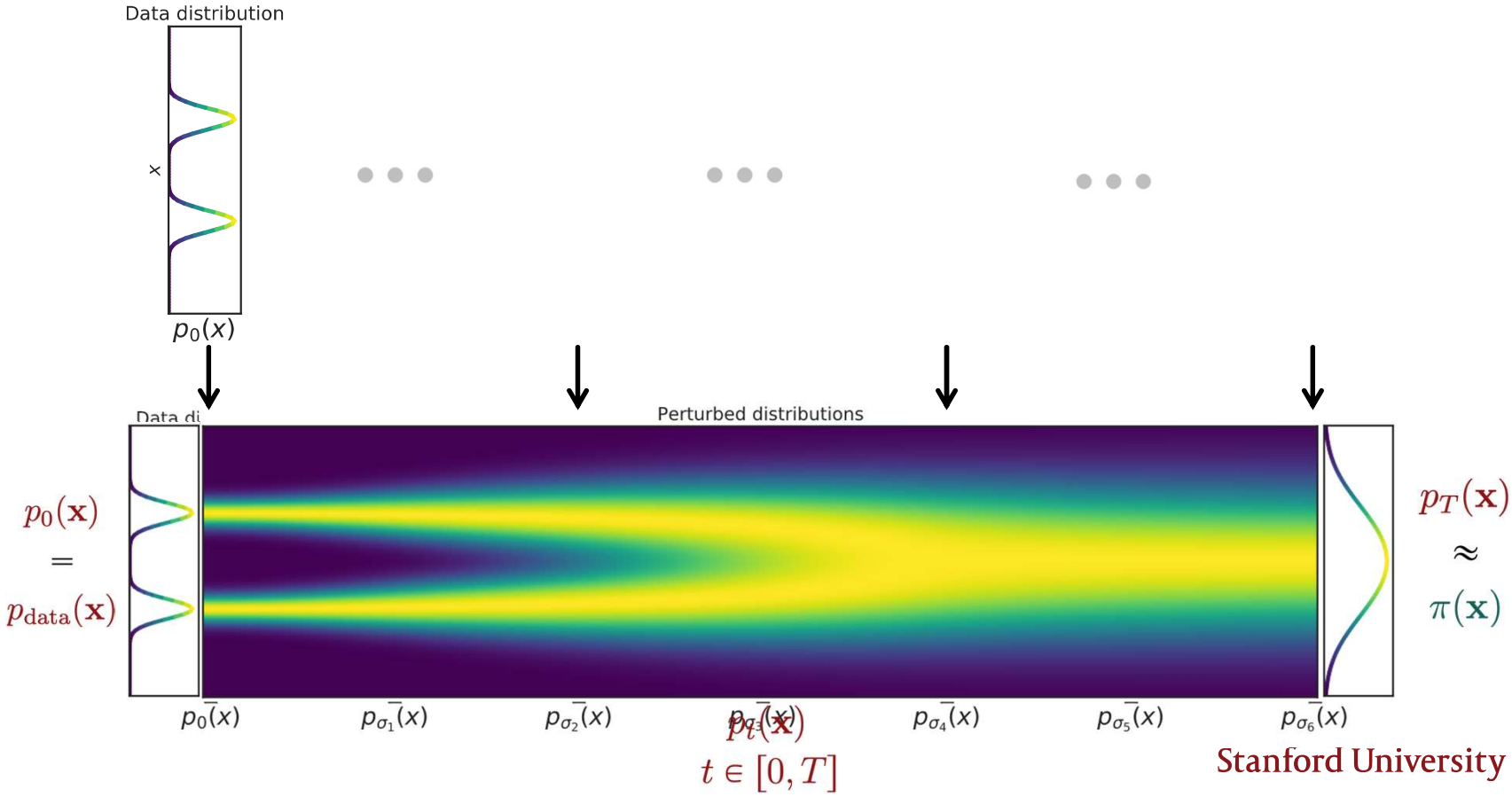
Experiments: sampling

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

High Resolution Image Generation



Infinite noise levels



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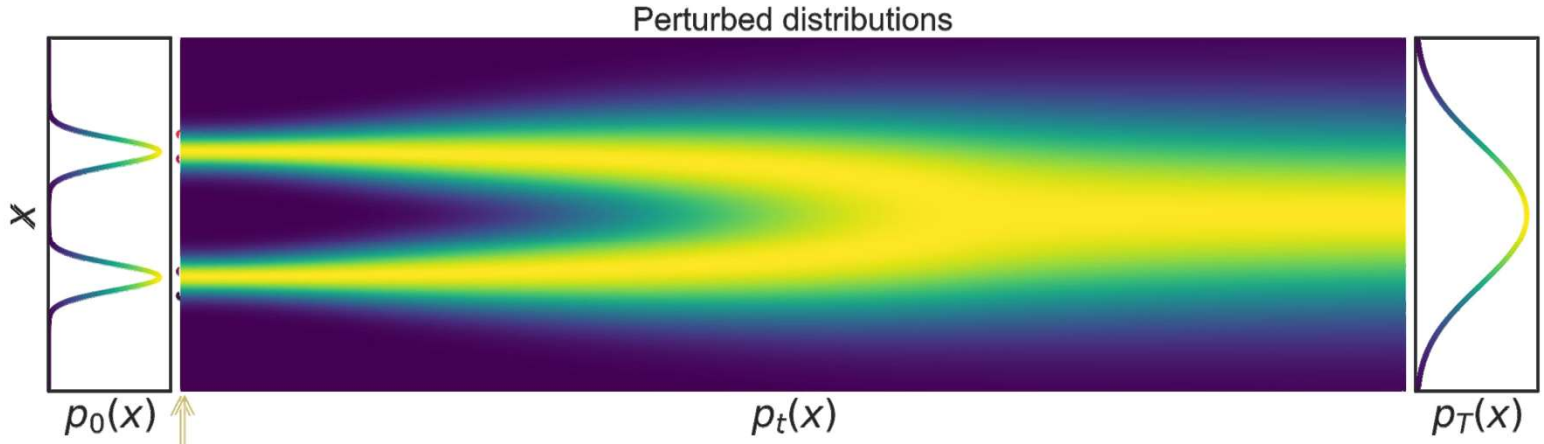
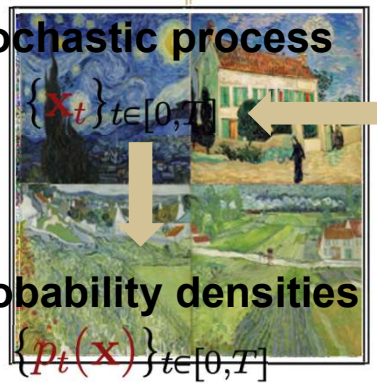
Perturbing data with stochastic processes



Stochastic process



Probability densities

Stochastic differential equation (SDE)

$$\mathrm{d}\mathbf{x}_t = \boldsymbol{f}(\mathbf{x}_t, t)\,\mathrm{d}t + g(t)\,\mathrm{d}\mathbf{w}_t$$

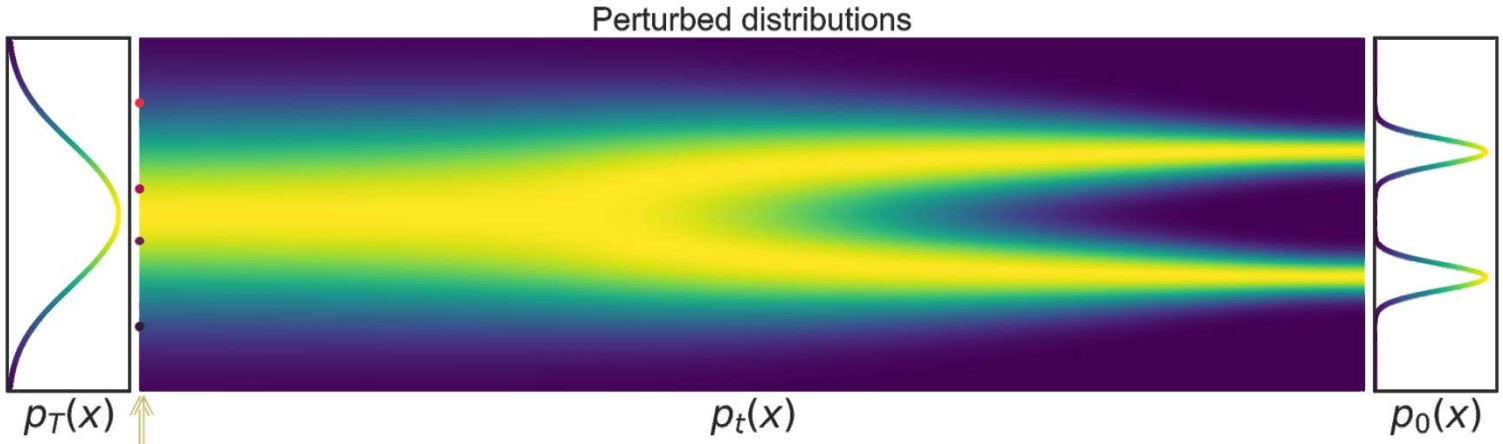
Deterministic drift — Infinitesimal noise

WLOG: Toy SDE

$$\mathrm{d}\mathbf{x}_t = \sigma(t)\,\mathrm{d}\mathbf{w}_t$$

$$p_T(\mathbf{x}) \approx \pi(\mathbf{x})$$

Generation via reverse stochastic processes



$$\pi(\mathbf{x}) \approx p_T(\mathbf{x})$$

Forward SDE (t: 0→T)

$$\mathrm{d}\mathbf{x}_t = \sigma(t)\,\mathrm{d}\mathbf{w}_t$$

Reverse SDE (t: T→0)

$$\mathrm{d}\mathbf{x}_t = -\sigma(t)^2 \nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t)\,\mathrm{d}t + \sigma(t)\,\mathrm{d}\bar{\mathbf{w}}_t$$

Infinitesimal noise in the reverse time direction

Score function!

Score-based generative modeling via SDEs

- Time-dependent score-based model

$$\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t) \approx \nabla_{\mathbf{x}} \log p_t(\mathbf{x})$$

- Training:

$$\mathbb{E}_{t \in \mathcal{U}(0,T)}[\lambda(t) \mathbb{E}_{p_t(\mathbf{x})}[\| \nabla_{\mathbf{x}} \log p_t(\mathbf{x}) - \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t) \|_2^2]]$$

- Reverse-time SDE

$$\mathrm{d}\mathbf{x} = -\sigma^2(t) \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t) \mathrm{d}t + \sigma(t) \mathrm{d}\bar{\mathbf{w}}$$

- Euler-Maruyama (analgous to Euler for ODEs)

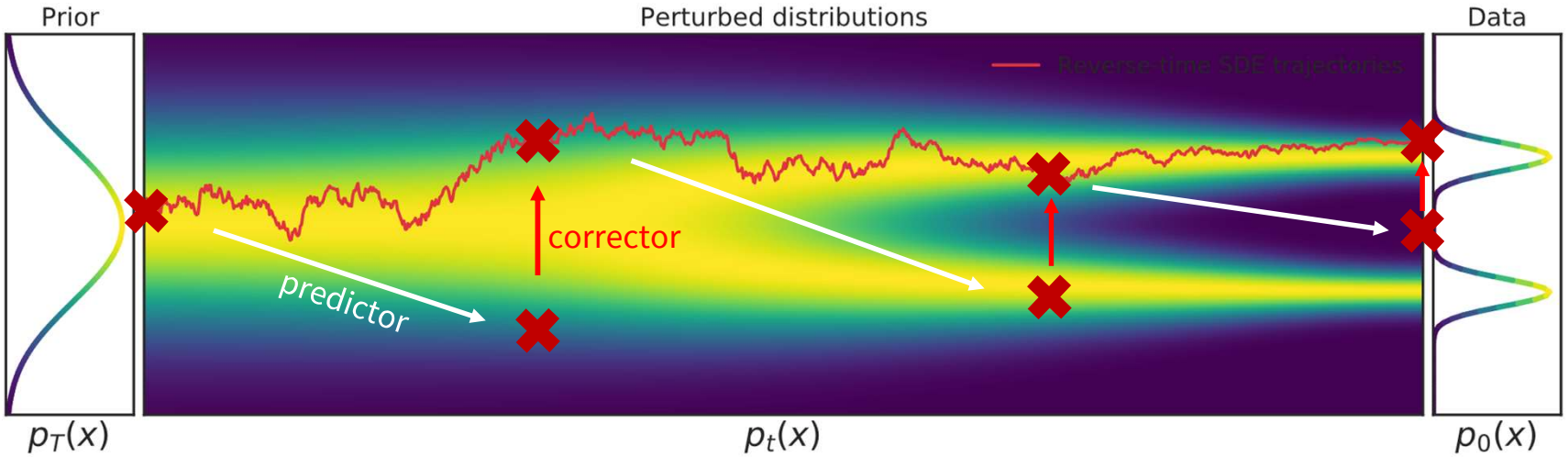
$$\mathbf{x} \leftarrow \mathbf{x} - \sigma(t)^2 \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}, t) \Delta t + \sigma(t)\ \mathbf{z} \quad (\mathbf{z} \sim \mathcal{N}(\mathbf{0}, |\Delta t|\ \mathbf{I}))$$

$$t \leftarrow t + \Delta t$$

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

Predictor-Corrector sampling methods

- Predictor-Corrector sampling.
  - **Predictor:** Numerical SDE solver
  - **Corrector:** Score-based MCMC



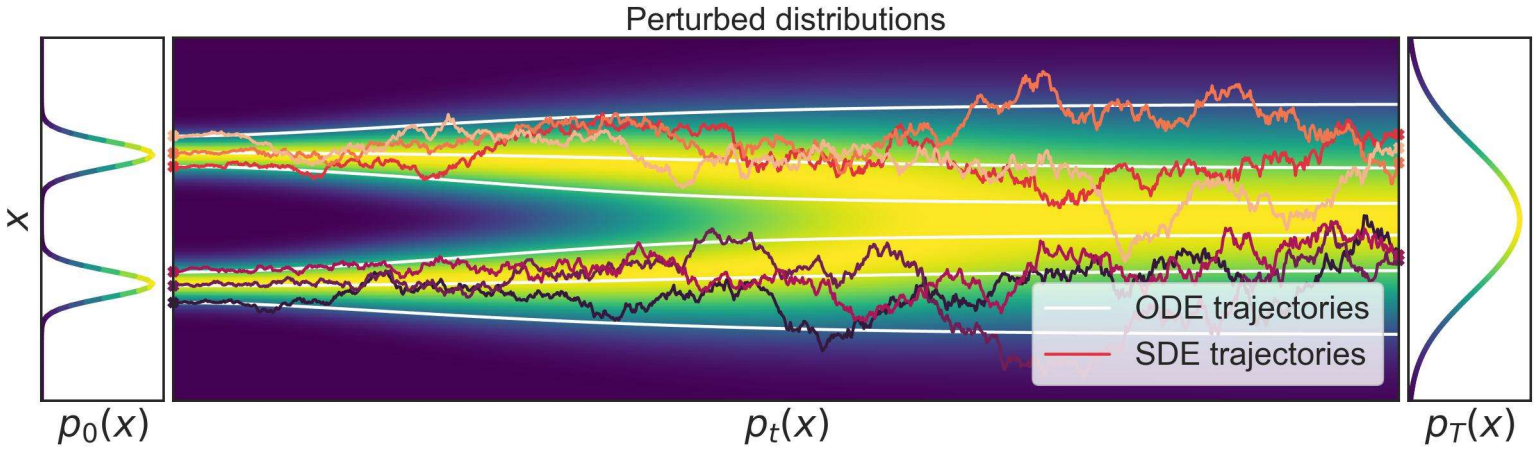
Results on predictor-corrector sampling

Model	FID↓	IS↑
Conditional		
BigGAN (Brock et al., 2018)	14.73	9.22
StyleGAN2-ADA (Karras et al., 2020a)	**2.42**	**10.14**
Unconditional		
StyleGAN2-ADA (Karras et al., 2020a)	2.92	9.83
NCSN (Song & Ermon, 2019)	25.32	8.87 ± .12
NCSNv2 (Song & Ermon, 2020)	10.87	8.40 ± .07
DDPM (Ho et al., 2020)	3.17	9.46 ± .11
DDPM++	2.78	9.64
DDPM++ cont. (VP)	2.55	9.58
DDPM++ cont. (sub-VP)	2.61	9.56
DDPM++ cont. (deep, VP)	2.41	9.68
DDPM++ cont. (deep, sub-VP)	2.41	9.57
NCSN++	2.45	9.73
NCSN++ cont. (VE)	2.38	9.83
NCSN++ cont. (deep, VE)	**2.20**	**9.89**

Song, Sohl-Dickstein, Kingma, Kumar, Ermon, Poole. “Score-Based Generative Modeling through Stochastic Differential Equations.” ICLR 2021.

High-Fidelity Generation for 1024x1024 Images

Converting the SDE to an ODE



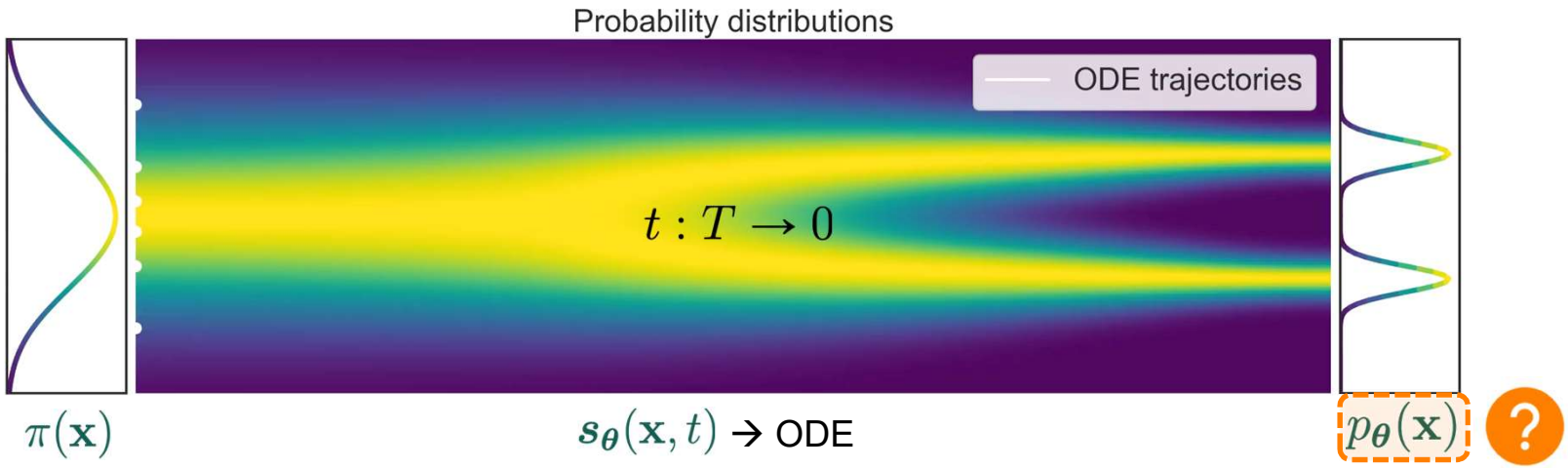
SDE **Ordinary differential equation (ODE)**

$$\mathrm{d}\mathbf{x}_t = \sigma(t)\,\mathrm{d}\mathbf{w}_t \quad \Longleftrightarrow \quad \frac{\mathrm{d}\mathbf{x}_t}{\mathrm{d}t} = -\frac{1}{2}\sigma(t)^2 \boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{x}_t)}$$

Score function

$$\approx \boldsymbol{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)$$

Evaluating the probabilities with ODEs



Computing the probability density function (change of variables formula)

$$\log p_{\boldsymbol{\theta}}(\mathbf{x}_0) = \log \pi(\mathbf{x}_T) - \frac{1}{2}\int_0^T \sigma(t)^2 \operatorname{trace}\left(\nabla_{\mathbf{x}} \boldsymbol{s}_{\boldsymbol{\theta}}(\mathbf{x}, t)\right) \mathrm{d}t$$

ODE solver

Computable in polynomial time

Unbiased estimator

It is a (continuous-time) normalizing flow model!

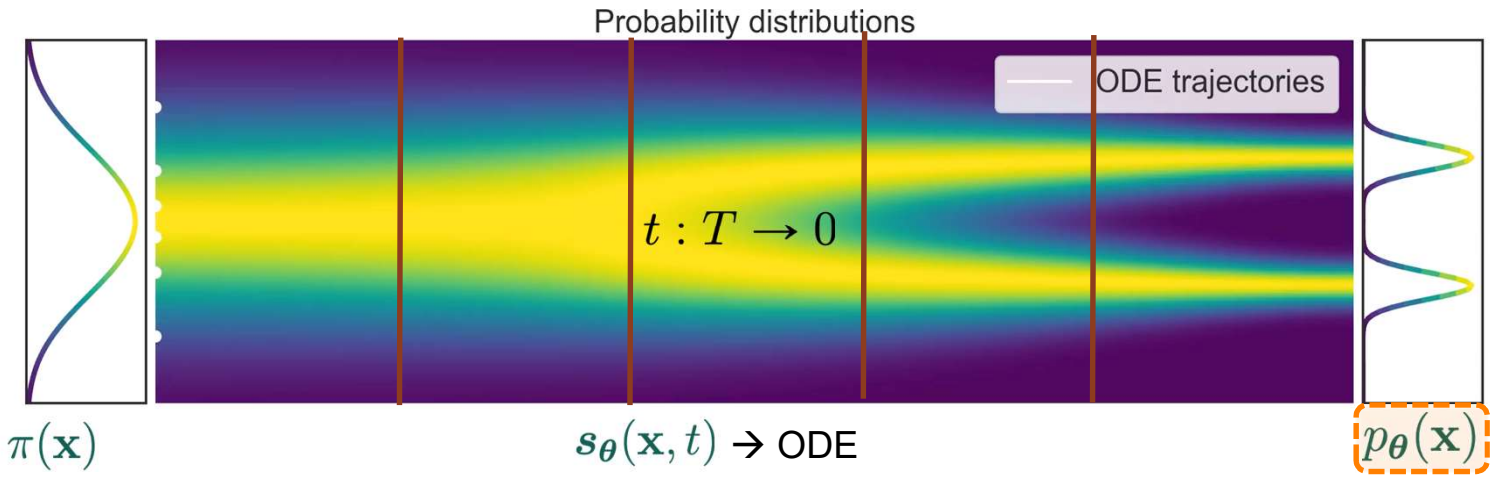
Achieving highest probabilities on test data

Negative log-probability ↓ (**bits/dim**)

Method	CIFAR-10	ImageNet 32x32
PixelSNAIL [Chen et al. 2018]	2.85	3.80
Delta-VAE [Razavi et al. 2019]	2.83	3.77
Sparse Transformer [Child et al. 2019]	2.80	–

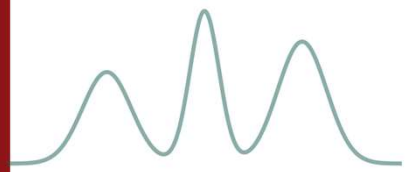
Challenges years of dominance of autoregressive models and VAEs

Accelerated sampling



- Numerical methods + ODE formulation to accelerate sampling
- DDIM [Song and Ermon, 2021]:
  - Coarsely discretize the time axis, take big steps
  - Corresponds to exponential integrator (semi-linear ODE) [Lu et al, 2022; Zhang and Chen, 2022]
  - 10x-50x speedups, comparable sample quality

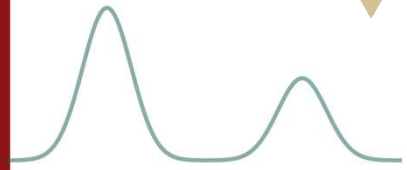
Control the generation process



$p(\mathbf{x})$

Forward model $p(\mathbf{y} \mid \mathbf{x})$

Control signal $\mathbf{y}$ = “dog”



$p(\mathbf{x} \mid \mathbf{y})$

Inverse distribution

Bayes’ rule:

$$p(\mathbf{x} \mid \mathbf{y}) = \frac{p(\mathbf{x})\, p(\mathbf{y} \mid \mathbf{x})}{p(\mathbf{y})}$$

Bayes’ rule for score functions:

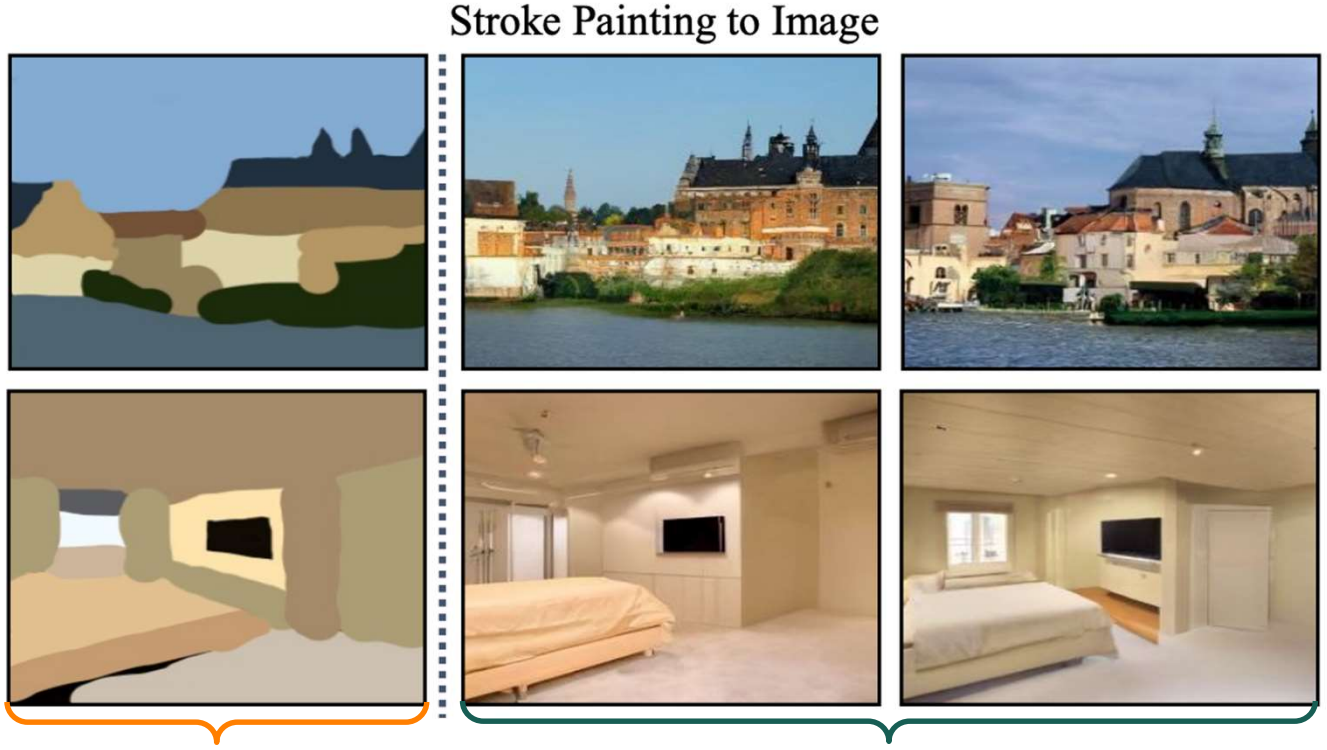
$$\nabla_{\mathbf{x}} \log p(\mathbf{x} \mid \mathbf{y}) = \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \nabla_{\mathbf{x}} \log p(\mathbf{y} \mid \mathbf{x}) - \nabla_{\mathbf{x}} \log p(\mathbf{y})$$

$$= \nabla_{\mathbf{x}} \log p(\mathbf{x}) + \nabla_{\mathbf{x}} \log p(\mathbf{y} \mid \mathbf{x})$$

$\nabla_{\mathbf{x}} \log p(\mathbf{y})$ → 0

Plug in different forward models for the same score model

Stroke to image synthesis



Stroke paintings

$\mathbf{y}$

Sampled images

$\mathbf{x} \mid \mathbf{y}$

Forward model

$p(\mathbf{y} \mid \mathbf{x})$

can be specified.

[Meng, He, Song, Song, Wu, Zhu, Ermon. ICLR 2022]

Language-guided image generation

$\mathbf{y}$

$\mathbf{x} \mid \mathbf{y}$

(Prompt)
Treehouse in the style of Studio Ghibli animation

Forward model

$p(\mathbf{y} \mid \mathbf{x})$

is an image captioning neural network.

[Work by @danielrussruss]

Controllable generation: Text-guided generation

An abstract painting of computer science:

A painting of the starry night by van Gogh

https://colab.research.google.com/drive/1FuOobQOmDJuG7rGsMWfQa883A9r4HxEO?usp=sharing

Conclusion

- **Gradients of distributions (scores) can be estimated easily**
  - **Flexible architecture choices** — no need to be normalized/invertible
  - **Stable training** — no minimax optimization
- **Better or comparable sample quality to GANs**
  - State-of-the-art performance on CIFAR-10 and others
  - Scalable to resolution of 1024x1024 for image generation
- **Exact likelihood computation**
  - State-of-the-art likelihood on CIFAR-10
  - Sample editing via manuplating latent codes