Generative Modeling by Estimating Gradients of the Data Distribution

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ABSTRACT

- We propose score-based generative modeling as a new framework for building generative models, where we first estimate the gradient of data distribution and then sample with Langevin dynamics.
- We analyze a straightforward implementation of score-based generative models and pinpoint several pitfalls.
- We propose the noise conditional score network (NCSN) and annealed Langevin dynamics to improve score-based generative modeling.
- Experimentally, we show that our approach can generate high quality images that were previously only produced by the best likelihood-based models or GANs. We achieve the new state-of-the-art inception score on CIFAR-10, and an FID score comparable to SNGANs.

Code:

SCORE-BASED GENERATIVE MODELING

Score Estimation:

$$\{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \overset{\text{i.i.d.}}{\sim} p_{\text{data}}(\mathbf{x})$$

$$\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) \quad \textbf{(Score)}$$

Densities — Samples — Scores

Score Matching (Hyvärinen 2005):

$$s_\theta(\mathbf{x}) : \mathbb{R}^D \to \mathbb{R}^D \quad \textbf{(Score Model)}$$

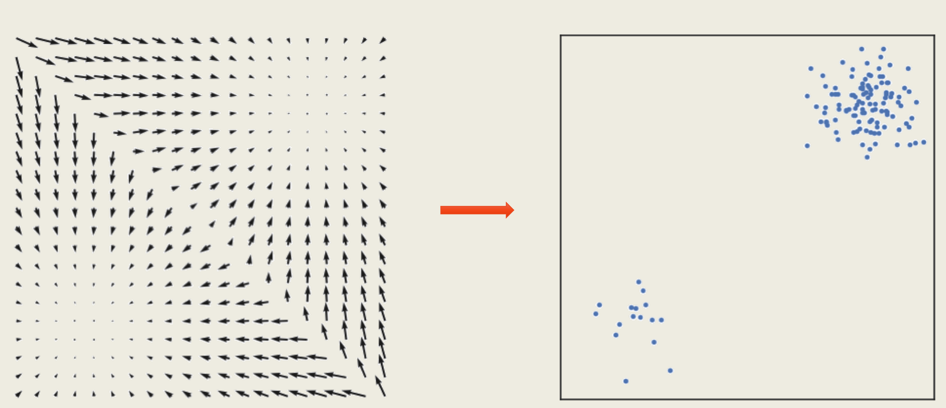
$$\frac{1}{2}\mathbb{E}_{p(\mathbf{x})}[\|\nabla_{\mathbf{x}} \log p(\mathbf{x}) ? - s_\theta(\mathbf{x})\|_2^2]$$

(integration by parts)

$$\mathbb{E}_{p(\mathbf{x})}\left[\frac{1}{2}\|s_\theta(\mathbf{x})\|_2^2 + \operatorname{tr}(\underbrace{\nabla_{\mathbf{x}} s_\theta(\mathbf{x})}_{\text{Jacobian of } s_\theta(\mathbf{x})})\right]$$

- Denoising Score Matching (Vincent 2010)
- Sliced Score Matching (Song et al. 2019)

Langevin dynamics:



Score Model — Samples

- Initialize $\tilde{\mathbf{x}}_0 \sim \pi(\mathbf{x})$
- Repeat for $t \leftarrow 1, 2, \cdots, T$

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

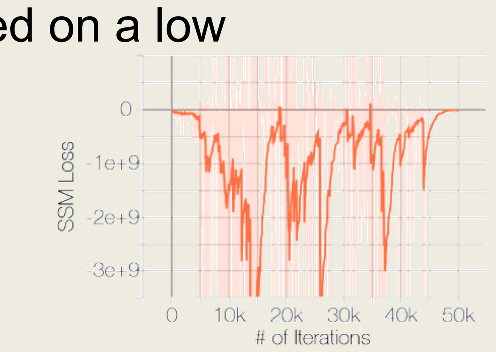
$$\tilde{\mathbf{x}}_t \leftarrow \tilde{\mathbf{x}}_{t-1} + \frac{\epsilon}{2}\nabla_{\mathbf{x}} \log p(\tilde{\mathbf{x}}_{t-1}) + \sqrt{\epsilon}\, \mathbf{z}_t$$

(approximate with $s_\theta(\mathbf{x})$!)

CHALLENGES OF SCORE-BASED GENERATIVE MODELING

Ill-defined Scores:

- The data distribution is supported on a low dimensional manifold
- The data distribution is discrete

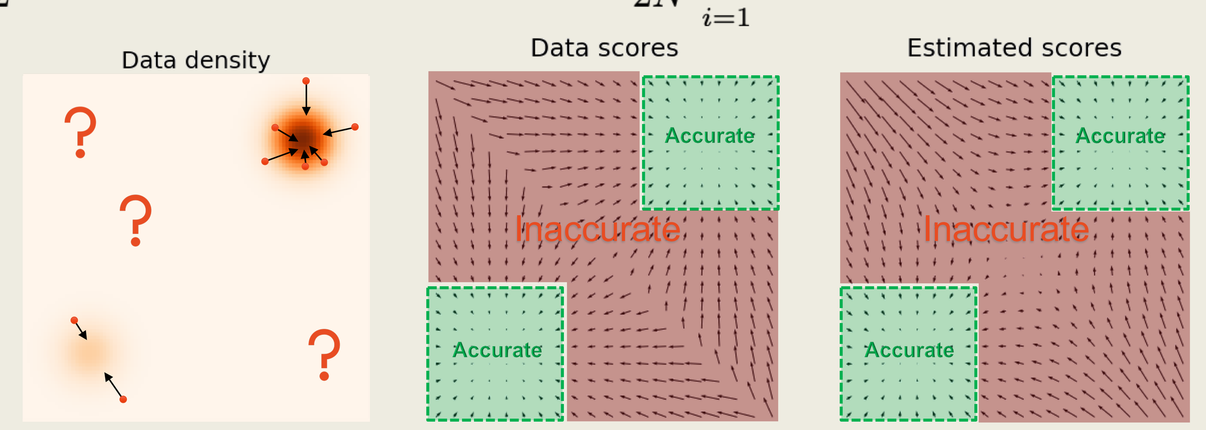


Unstable!

Low Data Density Regions:

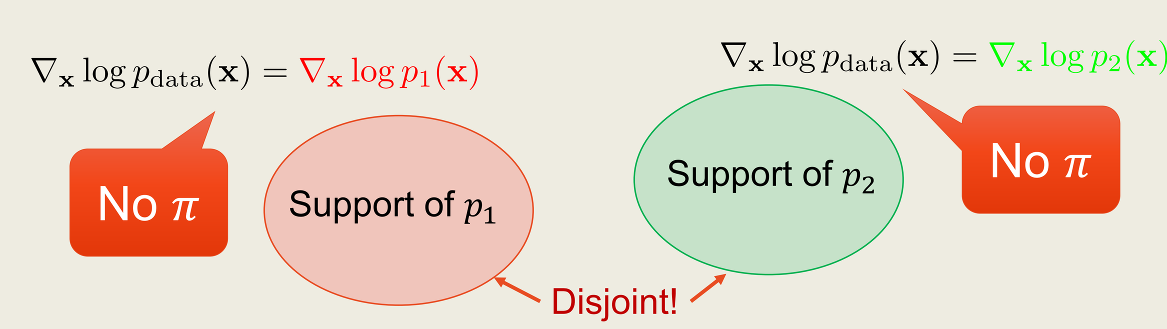
Inaccurate score estimation:

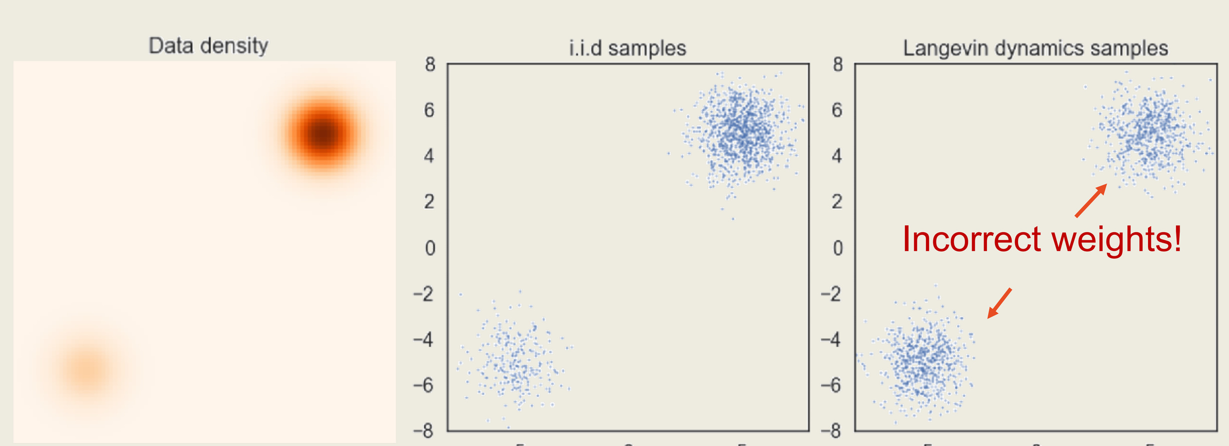
$$\frac{1}{2}\mathbb{E}_{p_{\text{data}}}[\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}) - s_\theta(\mathbf{x})\|_2^2] \approx \frac{1}{2N}\sum_{i=1}^{N}\|\nabla_{\mathbf{x}} \log p_{\text{data}}(\mathbf{x}_i) - s_\theta(\mathbf{x}_i)\|_2^2$$



Slow mixing of Langevin dynamics:

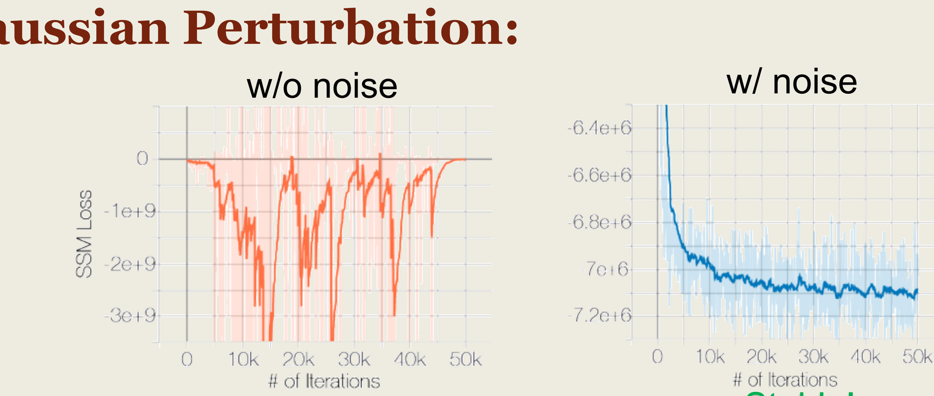
$$p_{\text{data}}(\mathbf{x}) = \pi p_1(\mathbf{x}) + (1-\pi) p_2(\mathbf{x})$$





NOISE CONDITIONAL SCORE NETWORKS

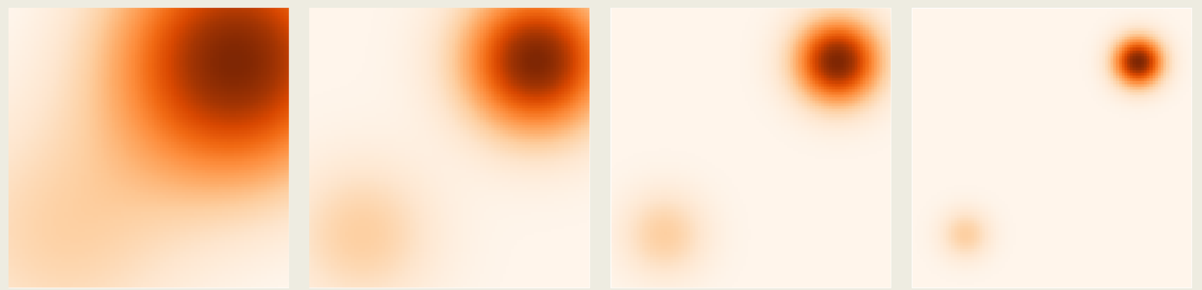
Gaussian Perturbation:



Unstable! — Stable!

Noise Conditional Score Networks (NCSN):

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



$$s_\theta(\mathbf{x}, \sigma) \quad \text{(NCSN)}$$

$$\mathcal{L}_{\{\sigma_i\}_{i=1}^L}(\theta) = \lambda(\sigma_1)\ell_{\sigma_1}(\theta) + \lambda(\sigma_2)\ell_{\sigma_2}(\theta) + \cdots + \lambda(\sigma_L)\ell_{\sigma_L}(\theta)$$

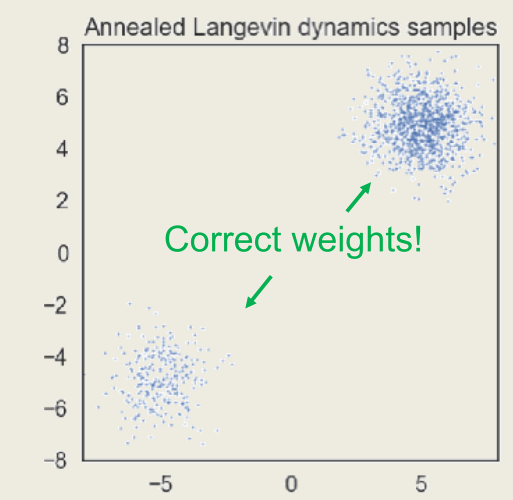
(Objective: mixture of score matching)

Annealed Langevin dynamics:

Algorithm 1 Annealed Langevin dynamics.

Require: $\{\sigma_i\}_{i=1}^L, \epsilon, T$.

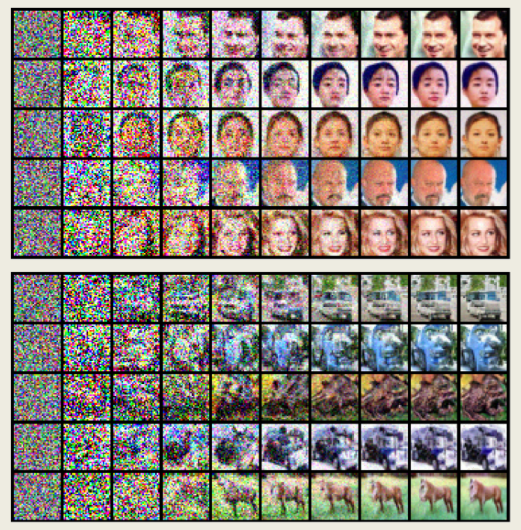
```
Initialize x̃_0
for i ← 1 to L do
    α_i ← ε · σ_i^2 / σ_L^2        ▷ α_i is the step size.
    for t ← 1 to T do
        Draw z_t ~ N(0, I)
        x̃_t ← x̃_{t−1} + (α_i/2) s_θ(x̃_{t−1}, σ_i) + √α_i z_t
    end for
    x̃_0 ← x̃_T
end for
return x̃_T
```



EXPERIMENTS

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**

Inception and FID scores



Sampling procedure

Inpainting CelebA images

Inpainting CIFAR-10 images