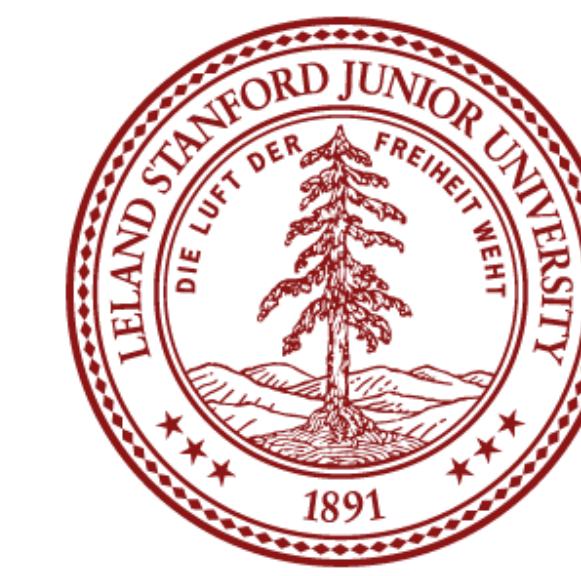


Improved Techniques for Training Score-Based Generative Models

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Overview

Score-based generative models [1] can produce high-quality samples comparable to GANs without requiring adversarial training.

How they work:

1. Perturb the data distribution with multiple scales of noise.
2. Jointly estimate the score (gradient of log probability density) of each noise-perturbed data distribution by training a noise-conditional model with score matching.
3. Generate samples by running Langevin MCMC on noise-conditional score models while gradually annealing down the noise scales.

Our contributions:

1. Theoretically-guided methods for choosing noise scales and setting the hyperparameters of Langevin MCMC.
2. Improve the performance of previous models, scaling the resolution of samples to 256 x 256.

Background

Score: $\nabla_{\mathbf{x}} \log p(\mathbf{x})$

Score-Based Model: $s_{\theta}(\mathbf{x}) \approx \nabla_{\mathbf{x}} \log p(\mathbf{x})$

Noise-Perturbed Distribution:

$$p_{\sigma}(\mathbf{x}) := \int p(\mathbf{x}') \mathcal{N}(\mathbf{x}; \mathbf{x}', \sigma^2 \mathbf{I}) d\mathbf{x}'$$

Noise-Conditional Score-Based Model: $s_{\theta}(\mathbf{x}, \sigma) \approx \nabla_{\mathbf{x}} \log p_{\sigma}(\mathbf{x})$

Multiple Scales of Noise Perturbation:

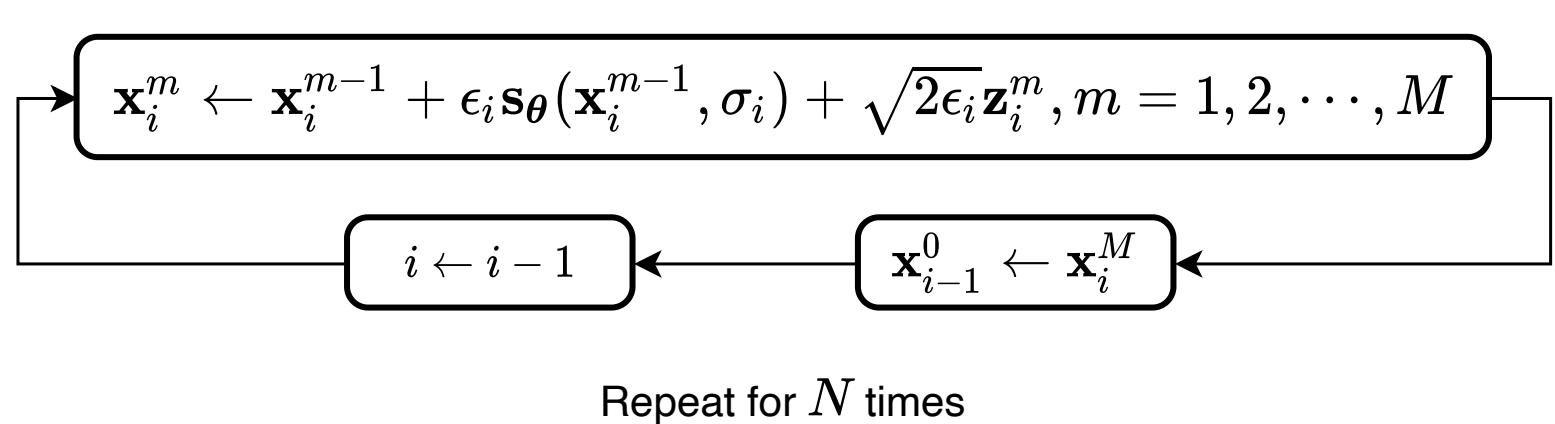
$$\sigma_1 < \sigma_2 < \dots < \sigma_N$$

$$s_{\theta}(\mathbf{x}, \sigma_i) \approx \nabla_{\mathbf{x}} \log p_{\sigma_i}(\mathbf{x}), \quad i = 1, 2, \dots, N$$

Training:

$$\frac{1}{2N} \sum_{i=1}^N \underbrace{\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \mathbb{E}_{\mathcal{N}(\tilde{\mathbf{x}}; \mathbf{x}, \sigma_i^2 \mathbf{I})} \left[\left\| \sigma_i s_{\theta}(\tilde{\mathbf{x}}, \sigma_i) + \frac{\tilde{\mathbf{x}} - \mathbf{x}}{\sigma_i} \right\|_2^2 \right]}_{\text{denoising score matching}}$$

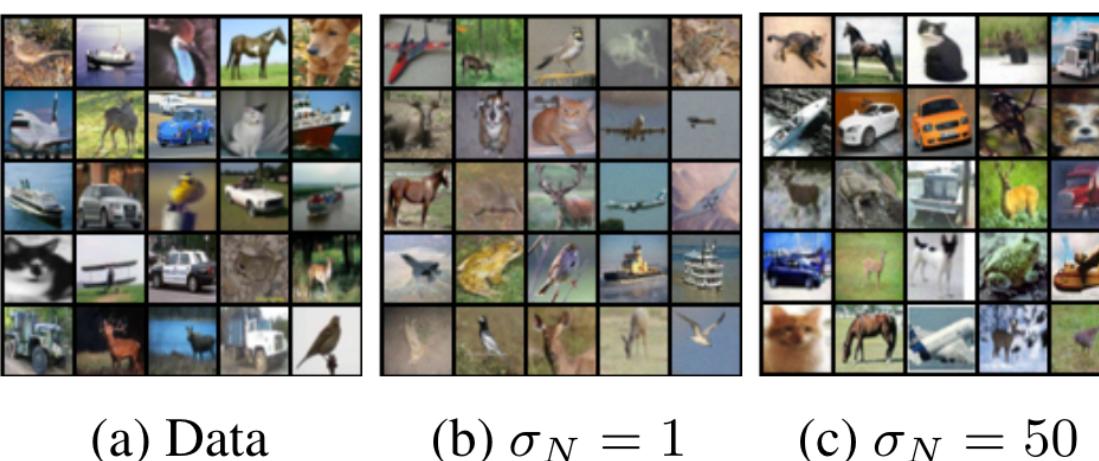
Annealed Langevin dynamics:



Choosing Noise Scales

Initial Noise Scale: σ_N

Theoretical analysis assuming data distribution is a mixture of Gaussian:



Sampling from a mixture of Gaussian centered at test images with annealed Langevin dynamics using different initial noise scales.

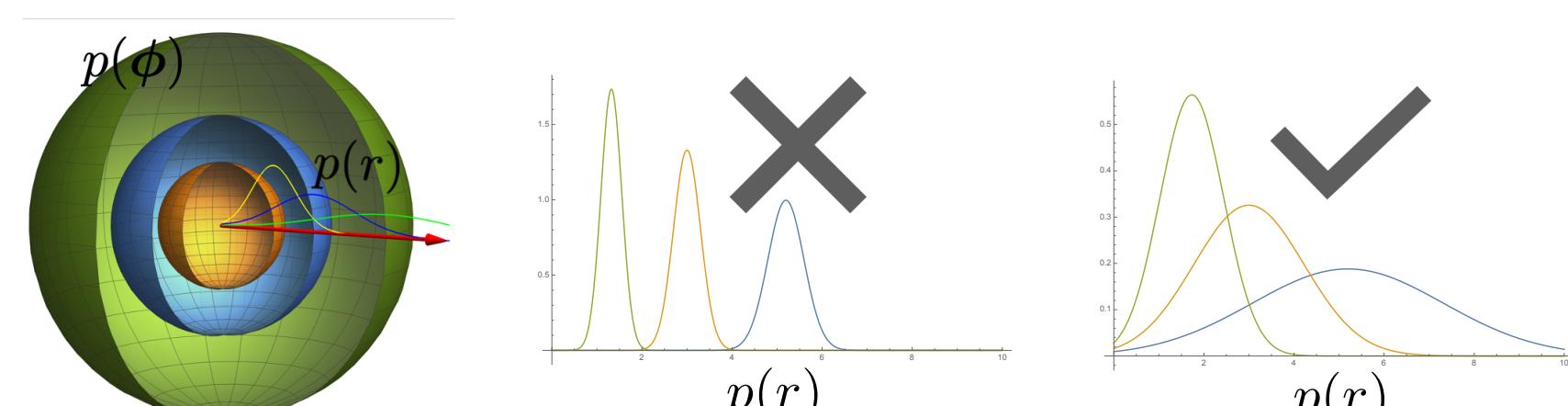
Technique 1 (Initial noise scale). Choose σ_N to be as large as the maximum Euclidean distance between all pairs of training data points.

Final Noise Scale: $\sigma_1 = 0.01$ (small enough to make the smallest noise-perturbed data distribution indiscernable from clean data)

Other Noise Scales: choose N and $\sigma_2 < \sigma_3 < \dots < \sigma_{N-1}$

Intuition: adjacent noise-perturbed distributions should have sufficient **overlap**.

Analysis: assuming data distribution is a single Gaussian.



Technique 2 (Other noise scales). Choose $\{\sigma_i\}_{i=1}^N$ as a geometric progression with common ratio γ , such that $\Phi(\sqrt{2D}(\gamma - 1) + 3\gamma) - \Phi(\sqrt{2D}(\gamma - 1) - 3\gamma) \approx 0.5$.

Configuring Annealed Langevin Dynamics

Theoretical analysis assuming data distribution is a single Gaussian.

Proposition 3. Let $\gamma = \frac{\sigma_i}{\sigma_{i-1}}$, and we choose the step size $\epsilon_i = \epsilon \cdot \frac{\sigma_i^2}{\sigma_N^2}$. After running Langevin MCMC, we have the sample $\mathbf{x}^M \sim \mathcal{N}(\mathbf{0}, \sigma_i^2 \mathbf{I})$, where

$$\frac{\sigma_i^2}{\sigma_N^2} = \left(1 - \frac{\epsilon}{\sigma_N^2}\right)^{2M} \left(\gamma^2 - \frac{2\epsilon}{\sigma_N^2 - \sigma_N^2 \left(1 - \frac{\epsilon}{\sigma_N^2}\right)^2} \right) + \frac{2\epsilon}{\sigma_N^2 - \sigma_N^2 \left(1 - \frac{\epsilon}{\sigma_N^2}\right)^2}.$$

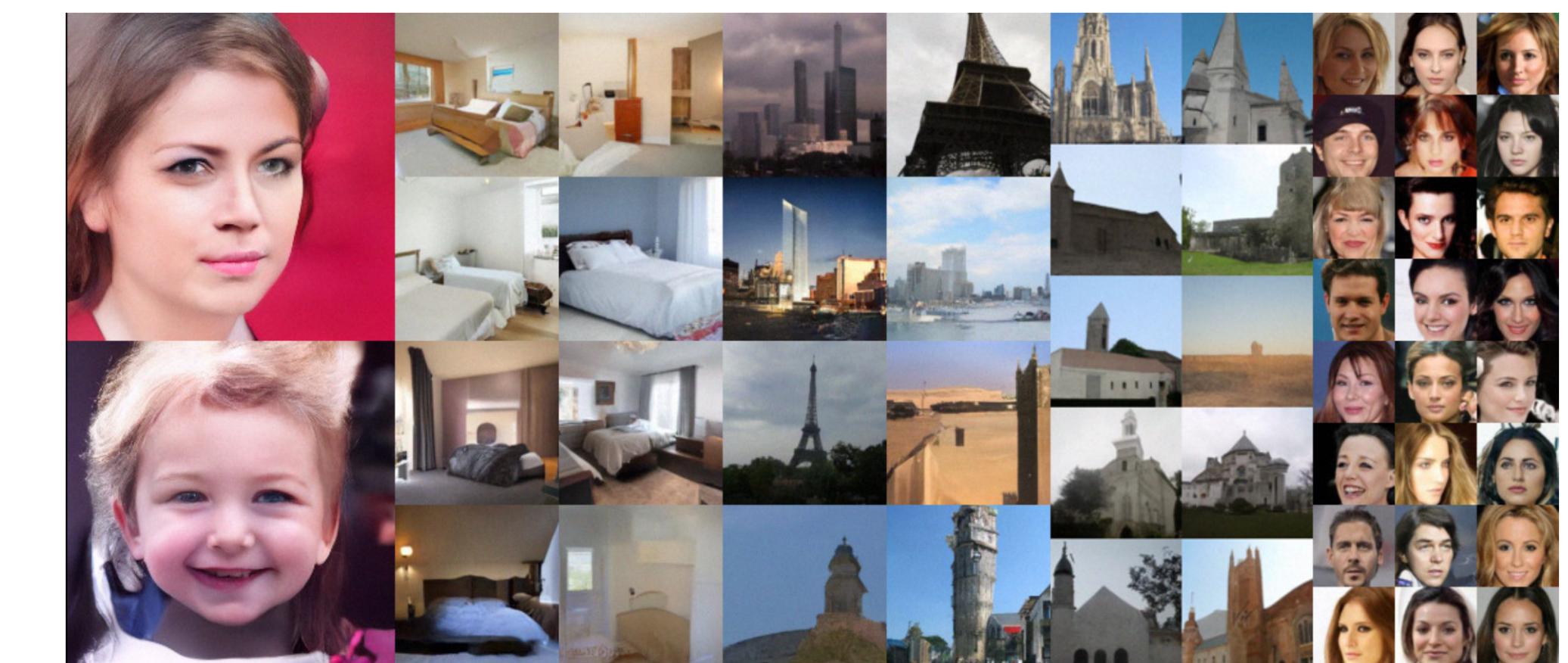
Technique 4 (selecting M and ϵ). Choose M as large as allowed by a computing budget and then select an ϵ that makes $\frac{\sigma_i^2}{\sigma_N^2}$ maximally close to 1.

Other Improved Techniques

Technique 3 (Noise conditioning). Parameterize the NCSN with $s_{\theta}(\mathbf{x}, \sigma) = s_{\theta}(\mathbf{x})/\sigma$, where s_{θ} is an unconditional score network.

Technique 5 (EMA). Apply exponential moving average to parameters when sampling.

Experimental Results



Model	Inception ↑	FID ↓
CIFAR-10 Unconditional		
PixelCNN [17]	4.60	65.93
IGEBM [18]	6.02	40.58
WGANGP [19]	7.86 ± .07	36.4
SNGAN [20]	8.22 ± .05	21.7
NCSN [1]	8.87 ± .12	25.32
NCSN (w/ denoising)	7.32 ± .12	29.8
NCSNv2 (w/o denoising)	8.73 ± .13	31.75
NCSNv2 (w/ denoising) [2]	8.40 ± .07	10.87
CelebA 64 × 64		
NCSN (w/o denoising)	-	26.89
NCSN (w/ denoising) [2]	-	25.30
NCSNv2 (w/o denoising)	-	28.86
NCSNv2 (w/ denoising) [2]	-	10.23

References

- [1] Song, Y. and Ermon, S., 2019. Generative modeling by estimating gradients of the data distribution. In Advances in Neural Information Processing Systems (pp. 11918-11930).
- [2] Jolicoeur-Martineau, A., Piché-Taillefer, R., Combes, R.T.D. and Mitliagkas, I., 2020. Adversarial score matching and improved sampling for image generation. In arXiv preprint arXiv:2009.05475.

