Denoising Score Matching and Diffusion Models

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Goal and approach

We aim to generate new samples from an unknown distribution given only observed data. For example, given a dataset of face images, we want to synthesize realistic unseen faces. Our approach has two steps:

- Learn the *score* of the data distribution, i.e. $\nabla_x \log p(x)$.
- Generate samples using either Langevin-based MCMC or SDE-based samplers.

Score matching

Suppose we are trying to learn a distribution $p(x) = \frac{e^{-f(x)}}{Z}$. The main problem with learning a distribution is its normalizing constant. Often, it is easy to learn a distribution up to a normalizing constant, and computing this constant can be very hard in a high-dimensional problem.
To bypass this constant, we instead try to learn its score, which does not depend on Z.

Sampling (naive Langevin dynamics)

Suppose we know the score field of a distribution, or we have trained a score network s_θ to approximate it (as we will explain later using Eq (2)). How do we actually draw samples from the distribution? The answer: Langevin dynamics!

$$x_{t+1} = x_t + \tau \nabla_x \log p(x_t) + \sqrt{2\tau}\, z_t, \qquad z_t \sim \mathcal{N}(0, I_d) \tag{1}$$

However, for multimodal data such as a Gaussian mixture, this naive approach often fails:

- Far from the data, the score can be undefined.
- The chain quickly collapses to a nearby mode and rarely crosses low-density regions.

This motivates learning and sampling from *smoothed* distributions p_σ obtained by adding Gaussian noise.

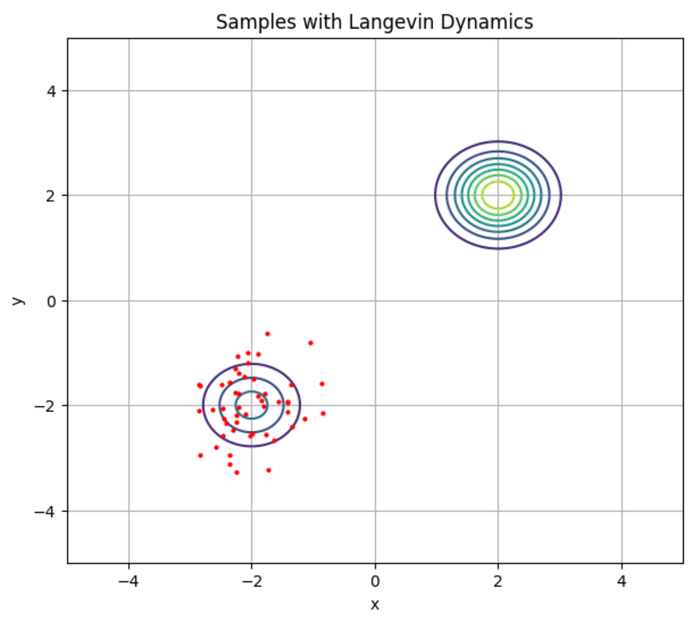


Fig. 1: Langevin dynamics fails to sample from a GMM.

Noise perturbation and score matching

More specifically, suppose we have an underlying data distribution $p(x)$ and consider a sequence of noise scales $\{\sigma_i\}_{i=1}^L$ such that $\sigma_1 > \sigma_2 > \cdots > \sigma_L$. For any $\sigma > 0$, define the Gaussian perturbation kernel

$$p_\sigma(\tilde{x} \mid x) = \mathcal{N}(\tilde{x} \mid x, \sigma^2 I_d)$$

and the corresponding perturbed distribution

$$p_\sigma(\tilde{x}) = \int p_\sigma(\tilde{x} \mid x)\, p(x)\, \mathrm{d}x$$

We train a noise-conditional score network $s_\theta(\tilde{x}, \sigma) \approx \nabla_{\tilde{x}} \log p_\sigma(\tilde{x})$ using denoising score matching:

$$\mathcal{L}(\theta) = \frac{1}{2L} \sum_{i=1}^{L} \mathbb{E}_{x\sim p}\, \mathbb{E}_{\tilde{x}\sim p_{\sigma_i}(\cdot|x)} \left[\left\| s_\theta(\tilde{x}, \sigma_i) - \nabla_{\tilde{x}} \log p_{\sigma_i}(\tilde{x} \mid x) \right\|_2^2 \right] \tag{2}$$

Since $p_{\sigma_i}(\tilde{x} \mid x)$ is Gaussian,

$$\nabla_{\tilde{x}} \log p_{\sigma_i}(\tilde{x} \mid x) = \frac{x - \tilde{x}}{\sigma_i^2}$$

so the target is available in closed form.

Bibliography

[1] A. Hyvärinen. *Estimation of Non-Normalized Statistical Models by Score Matching.* JMLR, 2005.

[2] Y. Song and S. Ermon. *Generative Modeling by Estimating Gradients of the Data Distribution.* NeurIPS, 2019.

[3] Y. Song et al. *Score-Based Generative Modeling through Stochastic Differential Equations.* ICLR, 2021.

[4] P. Vincent. *A Connection Between Score Matching and Denoising Autoencoders.* Neural Computation, 2011.

Annealed Langevin Dynamics

Once we have trained a noise-conditional score network $s_\theta(x, \sigma) \approx \nabla_x \log p_\sigma(x)$, we can sample by starting from a large noise level and progressively decreasing σ. This is *Annealed Langevin Dynamics*.
For a geometric noise schedule $\sigma_1 > \sigma_2 > \cdots > \sigma_L$, the sampler reads:

Algorithm: Annealed Langevin Dynamics

Require: $\{\sigma_i\}_{i=1}^L$, ϵ, T

```
Initialize x̃_0
for i ← 1 to L do
    τ_i ← ε · σ_i^2 / σ_L^2
    for t ← 1 to T do
        Draw z_t ~ N(0, I)
        x̃_t ← x̃_{t-1} + τ_i s_θ(x̃_{t-1}, σ_i) + √(2τ_i) z_t
    end for
    x̃_0 ← x̃_T
end for
return x̃_T
```

This combination of denoising score matching (2) and Annealed Langevin dynamics is known as the SMLD framework.

SDE

This problem can also be formulated with stochastic differential equations. Starting from a point x_0 in the data distribution, we can progressively add noise to it.
With $g(t) = \sqrt{2\,log\,\sigma}\,\sigma^t$, the forward process is written:

$$dx_t = g(t) dw_t$$

We can then train a time-dependent neural network with the following loss by simulating the time-forward SDE:

$$\mathcal{L}_{\mathrm{SDE}}(\theta) = \mathbb{E}_{t\sim\mathcal{U}[0,T]} \left[\lambda(t)\, \mathbb{E}_{x_0\sim p} \mathbb{E}_{x_t\sim p_{0t}(\,\cdot\,|x_0)} \left\| s_\theta(x_t, t) - \nabla_{x_t} \log p_{0t}(x_t \mid x_0) \right\|_2^2 \right] \tag{3}$$

To simulate a new sample, we now have to simulate the SDE:

$$\mathrm{d}x_t = -g(t)^2 s_{\theta^\star}(x_t, t)\, \mathrm{d}t + g(t)\, \mathrm{d}\bar{w}_t$$

In practice, this is done by with by simulating the equation by discretizing it.

Signal-To-Noise ratio

Rather than tuning the step size in the Annealed Langevin Dynamics, we can adjust the Signal-To-Noise ratio, which is defined as:

$$\mathrm{SNR}^2(x^{(k)}, \sigma; \tau) = \frac{\|\Delta x_{\mathrm{det}}\|_2^2}{\mathbb{E}\|\Delta x_{\mathrm{noise}}\|_2^2} = \frac{\|\tau\, s_\theta(x^{(k)}, \sigma)\|_2^2}{2\tau\, \mathbb{E}\|z^{(k)}\|_2^2} = \frac{\tau\, \|s_\theta(x^{(k)}, \sigma)\|_2^2}{2d}$$

Fixing a target $SNR(x^{(k)}, \sigma; \tau) = \rho$ yields an adaptive step size $\tau(x^{(k)}, \sigma) = \frac{2d\,\rho^2}{\|s_\theta(x^{(k)}, \sigma)\|_2^2}$

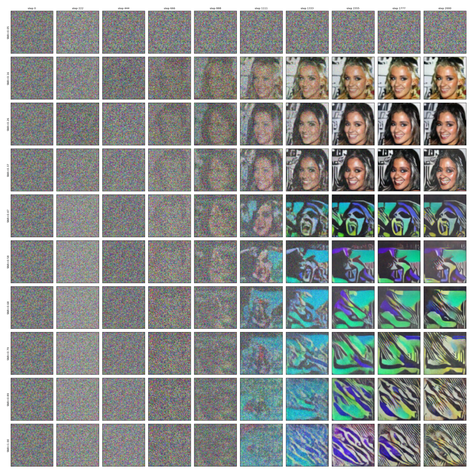
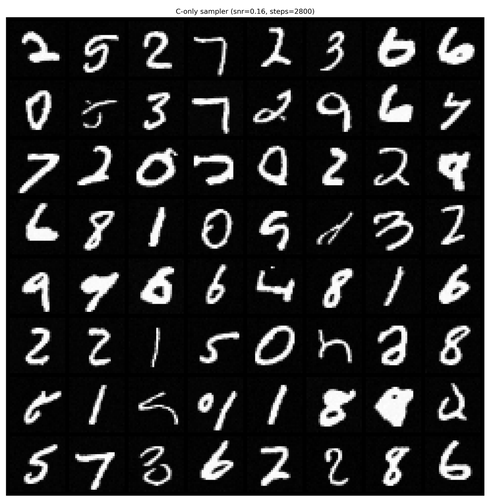


Fig. 2: Different trajectories, with SNR varying between 0.05 (top) and 1 (bottom)

Results

CelebA



MNIST (SMLD)

Fig. 3: Image sampling results (left: VE-SDE/PC on CelebA, right: SMLD on MNIST).

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