Introduction to SDE training and sampling

Justin T Chiu

July 27, 2023

Goals

2. How do we sample?

3. How do we train?

Setup

- Sampling requires solving the reverse SDE
- Solving the reverse SDE requires training a score model

Sampling by solving the reverse SDE

- Reverse SDE

$$dx = [f(x,t) - g(t)^2 \nabla_x \log p_t(x)]dt + g(t)dw$$

- w is Brownian motion (backward in time)
- dt is a negative time increment
- We have f and g from the forward SDE, which is defined by user
- Need trained time-dependent score score $s(x,t) \approx \nabla_x \log p_t(x)$

Euler-Maruyama solver

- Simplest SDE solver is Euler-Maruyama
- Discretize $[0, 1]$ into T steps
- Follow reverse SDE dynamics + a little Gaussian noise z_t (resembles Langevin dynamics)

$$\delta x \leftarrow [f(x,t) - g^2(t)s(x,t)]\delta t + g(t)\sqrt{|\delta t|}z_t$$
$$x \leftarrow x + \delta x$$
$$t \leftarrow t + \delta t$$

- Langevin dynamics for comparison: $x \leftarrow x + \text{scale} * s(x,t) + \text{other scale} * z_t$

Euler-Maruyama + predictor corrector illustration

Other solvers

- Other solvers don't fix a discretization
- Have resulted in improved image generation quality

Onto training

- The main missing piece is the score function $s(x, t) \approx \nabla_x \log p_t(x)$
- Training looks really close to score matching

Training: Quick review of score matching

- Start with image x_0
- Have I noise scales σ_i to perturb original image x_0
- Use score-matching to train score function at perturbed x' given x_0 and σ_i

$$\sum_i \sigma_i^2 E_{p_{data}(x)} E_{p_{\sigma_i}}(x'|x) \| s(x', \sigma_i) - \nabla_{x'} \log p_{\sigma_i}(x'|x) \|$$

SDE score training

- Score matching objective

$$\sum_i \sigma_i^2 E_{p_{data}(x)} E_{p_{\sigma_i}}(x'|x) \| s(x', \sigma_i) - \nabla_{x'} \log p_{\sigma_i}(x'|x) \|$$

- SDE training objective

$$E_{t \sim U(0,1)} E_{x(0)} E_{x(t)|x(0)} \lambda(t) \cdot \| s(x, t) - \nabla_x \log p_{0t}(x(t)|x(0)) \|_2^2$$

- How do we get $x(t)|x(0)$? Solve forward noising SDE, which was manually defined w/o learnable components