Stochastic Differential Equations for Generative Modeling

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May 2022

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GAN

$$L_D = -\mathbb{E}_{x\sim p_{data}}[\log D(x)] - \mathbb{E}_{z\sim p_z}[\log(1 - D(G(z))]$$
$$L_G = -\mathbb{E}_{z\sim p_z}[\log D(G(z))]$$

GAN as Energy Based Model

Assume that Discriminator is suboptimal, i.e. $D = D^*$

$$D(x) = \operatorname{logit}(d(x)) = \frac{1}{1 + \exp(-d(x))} \approx \frac{p_d(x)}{p_d(x) + p_g(x)} = \frac{1}{1 + p_g(x)/p_d(x)}$$

Thus,

$$p_d^*(x) = p_g(x)e^{d(x)}/K = \exp\left(-(-\log p_g(x) - d(x))\right)/K$$

Energy Function. Boltzmann distribution

$$p(z) = \exp(-E(z))/K$$

Thus, assuming that $x = G(z)$ one can obtain the following equation for Energy for GAN

$$E(z) = -\log p_0(z) - d(G(z))$$

Langevin Dynamics

$$z_{i+1} = z_i - \epsilon/2\nabla_z E(z) + \sqrt{\epsilon}n, n \sim N(0, I) \tag{1}$$

Input: N$\in \mathbf{N}_+$, $\epsilon > 0$
Output: Latent code $z_N \sim p_t(z)$
Sample $z_0 \sim p_0(z)$
for $i = 1$ **to** N **do**
$n_i \sim N(0, 1)$
$z_{i+1} = z_i - \epsilon/2\nabla_z E(z_i) + \sqrt{\epsilon}n_i$
end for

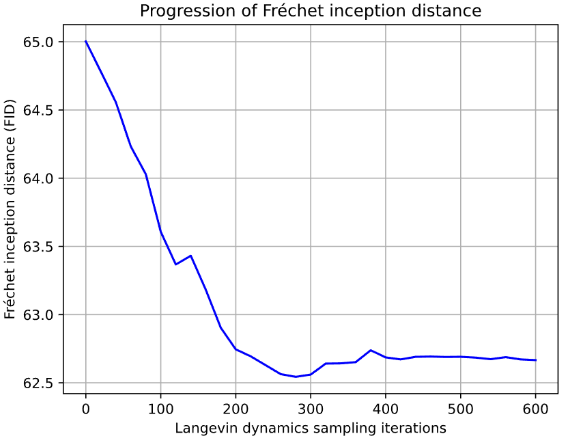
Frechet Inception Distance

FID can be calculated according to the following formula

$$d_F(\mu,\nu) := \left(\inf_{\gamma \in \Gamma(\mu,\nu)} \int_{\mathbb{R}^n \times \mathbb{R}^n} \|x - y\|^2 \, \mathrm{d}\gamma(x,y) \right)^{1/2}$$

Results

If one apply Langevin Dynamics for pretrained DCGAN on CIFAR10 we observe the following picture



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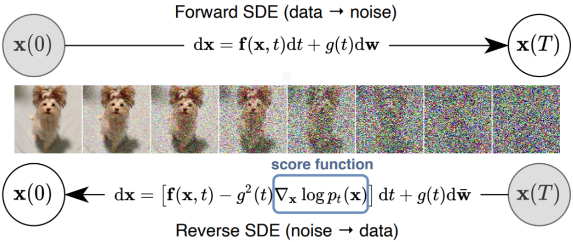
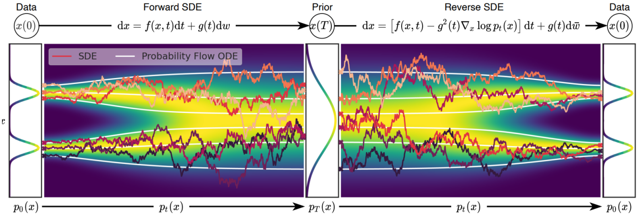
Score-based Generative Modelling through SDE

The core idea of the paper can be described via the following picture



Score-based Generative Modelling through SDE



The main problem is to fit the neural network $\mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t), t)$ such that

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

Loss function

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \mathbb{E}_t \left\{ \lambda(t) \mathbb{E}_{\mathbf{x}(0)} \mathbb{E}_{\mathbf{x}(t)|\mathbf{x}(0)} \left[\left\| \mathbf{s}_{\boldsymbol{\theta}}(\mathbf{x}(t), t) - \nabla_{\mathbf{x}(t)} \log p_{0t}(\mathbf{x}(t) \mid \mathbf{x}(0)) \right\|_2^2 \right] \right\}.$$

where

$$\lambda \propto 1/\mathbb{E}\left[\left\| \nabla_{\mathbf{x}(t)} \log p_{0t}(\mathbf{x}(t) \mid \mathbf{x}(0)) \right\|_2^2 \right]$$

2 approaches

In $\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$ functions $\mathbf{f}$ and g can be arbitrary, so we will consider 2 approaches

- Variance Exploding Approach
- Variance Preserving Approach

Variance Exploding

- SDE

$$\mathrm{d}\mathbf{x} = \sqrt{\frac{\mathrm{d}\left[\sigma^2(t)\right]}{\mathrm{d}t}}\,\mathrm{d}\mathbf{w}$$

- Forward Sampling

$$\mathbf{x}_i = \mathbf{x}_{i-1} + \sqrt{\sigma_i^2 - \sigma_{i-1}^2}\mathbf{z}_{i-1}$$

Variance Preserving

- SDE

$$d\mathbf{x} = -\frac{1}{2}\beta(t)\mathbf{x}dt + \sqrt{\beta(t)}d\mathbf{w}$$

- Forward Sampling

$$\mathbf{x}_i = \sqrt{1-\beta_i}\mathbf{x}_{i-1} + \sqrt{\beta_i}\mathbf{z}_{i-1}$$

Ancestral Sampling for Variance Preserving

$$\mathbf{x}_{i-1} = \frac{1}{\sqrt{1-\beta_i}} \left(\mathbf{x}_i + \beta_i \mathbf{s}_{\boldsymbol{\theta}^*} \left(\mathbf{x}_i, i \right) \right) + \sqrt{\beta_i} \mathbf{z}_i, \quad i = N, N-1, \cdots, 1$$

Reverse Diffusion

Given a forward SDE

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

and suppose the following iteration rule is a discretization of it:

$$\mathbf{x}_{i+1} = \mathbf{x}_i + \mathbf{f}_i\left(\mathbf{x}_i\right) + \mathbf{G}_i\mathbf{z}_i, \quad i = 0, 1, \cdots, N-1$$

Thus, one can propose to discretize the reverse-time SDE

$$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - \mathbf{G}(t)\mathbf{G}(t)^{\top}\nabla_{\mathbf{x}}\log p_t(\mathbf{x})\right]\mathrm{d}t + \mathbf{G}(t)\mathrm{d}\overline{\mathbf{w}}$$

which gives the following iteration rule for $i \in \{0, 1, \cdots, N-1\}$:

$$\mathbf{x}_i = \mathbf{x}_{i+1} - \mathbf{f}_{i+1}\left(\mathbf{x}_{i+1}\right) + \mathbf{G}_{i+1}\mathbf{G}_{i+1}^{\top}\mathbf{s}_{\boldsymbol{\theta}^*}\left(\mathbf{x}_{i+1}, i+1\right) + \mathbf{G}_{i+1}\mathbf{z}_{i+1},$$

where our trained score-based model $\mathbf{s}_{\boldsymbol{\theta}} * \left(\mathbf{x}_i, i\right)$.

Predictor-Corrector Sampling

Algorithm 2 PC sampling (VE SDE)

$\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \sigma_{\max}^2 \mathbf{I})$
for $i = N-1$ **to** 0 **do**
  $\mathbf{x}_i' \leftarrow \mathbf{x}_{i+1} + (\sigma_{i+1}^2 - \sigma_i^2)\mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_{i+1}, \sigma_{i+1})$
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{x}_i \leftarrow \mathbf{x}_i' + \sqrt{\sigma_{i+1}^2 - \sigma_i^2}\,\mathbf{z}$
  for $j = 1$ **to** M **do**
    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
    $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i, \sigma_i) + \sqrt{2\epsilon_i}\,\mathbf{z}$
return $\mathbf{x}_0$

Algorithm 3 PC sampling (VP SDE)

$\mathbf{x}_N \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
for $i = N-1$ **to** 0 **do**
  $\mathbf{x}_i' \leftarrow (2 - \sqrt{1 - \beta_{i+1}})\mathbf{x}_{i+1} + \beta_{i+1}\mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_{i+1}, i+1)$
  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
  $\mathbf{x}_i \leftarrow \mathbf{x}_i' + \sqrt{\beta_{i+1}}\,\mathbf{z}$
  Predictor
  for $j = 1$ **to** M **do**
  Corrector
    $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
    $\mathbf{x}_i \leftarrow \mathbf{x}_i + \epsilon_i \mathbf{s}_{\boldsymbol{\theta}^*}(\mathbf{x}_i, i) + \sqrt{2\epsilon_i}\,\mathbf{z}$
return $\mathbf{x}_0$

Results. FID on CIFAR10. VE

FID	P1000	P2000	**PC1000**
ancestral sampling	31.76	31.7	**30.57**
reverse diffusion	31.98	31.43	**30.96**

Results. FID on CIFAR10. VP

FID	P1000	P2000	**PC1000**
ancestral sampling	30.55	30.53	**29.74**
reverse diffusion	31.01	30.32	**30.01**