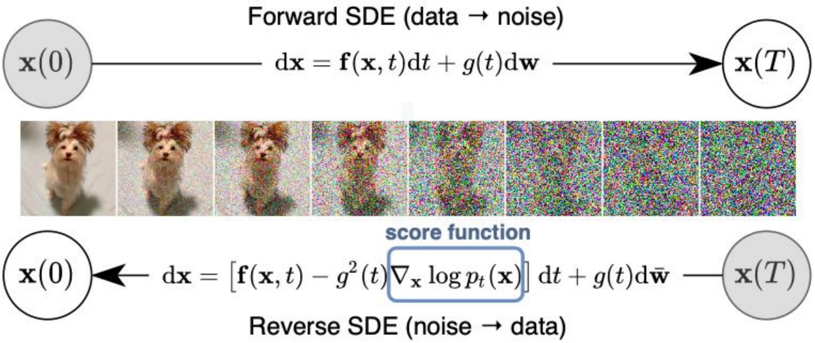
The Hidden Linear Structure in Score-Based Models and its Application

Daniil Shlenskii, Kseniia Petrushina, Arina Chumachenko, Bair Mikhailov, Nikita Kornilov

Skoltech

December 19, 2023

Score-based models intro



Score-based models intro

Goal

We want to sample from $p_{real}(\mathbf{x})$ which we don't know

Noising process (Forward process)

We set parameters of Forward SDE in a way, that marginal distributions have the following form.

$$p(\mathbf{x}, \sigma_t) = p_{real}(\mathbf{x}) * \mathcal{N}(\mathbf{x}|0, \sigma_t^2 I)$$

Denoising process(Backward process)

In that setup we can sample images using the following ODE which the same marginal distributions as aforementioned Reverse SDE.

$$d\mathbf{x} = -\dot{\sigma}_t \sigma_t \nabla_{\mathbf{x}} \log p(\mathbf{x}, \sigma_t) dt \quad (1)$$

Score-based models intro

Score function

We parameterize out score model in the follwing way:

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}, \sigma) \approx s_\theta(\mathbf{x}, \sigma) = \frac{D_\theta(\mathbf{x}, \sigma) - \mathbf{x}}{\sigma},$$

Where $D_\theta(\mathbf{x}, \sigma)$ is a prediction of a corresponding denoised object given σ and $x \sim p(\mathbf{x}, \sigma)$

Normal case

Analytical form

Let real data $p_{real}(\mathbf{x}) = \mathcal{N}(\mathbf{x}|\mu, \Sigma)$, then we have $p(\mathbf{x}, \sigma) = \mathcal{N}(\mathbf{x}|\mu, \Sigma + \sigma^2 I)$ and

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}, \sigma) = (\sigma^2 I + \Sigma)^{-1}(\mu - \mathbf{x})$$

Numerical linear algebra

Let positively semidefined Σ has rank r and by SVD decomposition $\Sigma = U\Lambda U^\top$, where orthogonal $U = [\mathbf{u}_1, \ldots, \mathbf{u}_r]$ and $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_r)$. This form and NLA help us to compute efficiently

$$(\sigma^2 I + \Sigma)^{-1} = \frac{1}{\sigma^2}(I + U\Lambda U^\top/\sigma^2)^{-1}$$

Effective computation

Woodbury matrix inversion

$$(I + AB)^{-1} = I - A(I + BA)^{-1}B$$

With $A = U, B = \Lambda U^\top/\sigma^2$ and orthogonal $U^\top U = I_r$ we get

$$\begin{aligned} (I + U\Lambda U^\top/\sigma^2)^{-1} &= (I - U\tilde{\Lambda}_\sigma U^\top) \\ \tilde{\Lambda}_\sigma &= \operatorname{diag}\left[\frac{\lambda_k}{\lambda_k + \sigma^2}\right] \end{aligned}$$

Finally,

$$\nabla_{\mathbf{x}} \log p(\mathbf{x}, \sigma) = \frac{1}{\sigma^2}(I - U\tilde{\Lambda}_\sigma U^\top)(\mu - \mathbf{x})$$

Effective computation

Solving ODE (1)

$$
\begin{aligned}
d\mathbf{x} &= -\sigma \nabla_{\mathbf{x}} \log p(\mathbf{x}, \sigma) \dot{\sigma} dt \\
d\mathbf{x} &= \frac{1}{\sigma}(I - U \tilde{\Lambda}_\sigma U^\top)(\mathbf{x} - \mu) d\sigma
\end{aligned}
$$

Let's find solution in basis U, i.e. $\mathbf{x} = \mu + \sum_{k=1}^{r} c_k(\sigma)\mathbf{u}_k$, where projection $c_k(\sigma) = \mathbf{u}_k^\top(\mathbf{x}(\sigma) - \mu)$. Then solve it for each k separately

$$
\frac{1}{\sigma}\left(1 - \frac{\lambda_k}{\lambda_k + \sigma^2}\right) = \frac{\sigma}{\lambda_k + \sigma^2} \implies dc_k(\sigma) = \frac{\sigma}{\lambda_k + \sigma^2} c_k(\sigma) d\sigma
$$

Effective computation

Solving ODE (1)

$$
\begin{aligned}
dc_k(\sigma) &= \frac{\sigma}{\lambda_k + \sigma^2} c_k(\sigma) d\sigma \\
d \log c_k(\sigma) &= d \log \sqrt{\lambda_k + \sigma^2} \\
c_k(\sigma) &= K \sqrt{\lambda_k + \sigma^2}
\end{aligned}
$$

Usually σ_T^2 is very large and $\mathcal{N}(\mathbf{x}|\mu, \sigma_T^2 I + \Sigma) \approx \mathcal{N}(0, \sigma_T^2 I)$. With initial condition $\mathbf{x}(T) = \mathbf{x}_T \sim \mathcal{N}(0, \sigma_T^2 I)$ we have

$$
c_k(\sigma_t) = \sqrt{\frac{\lambda_k + \sigma_t^2}{\lambda_k + \sigma_T^2}} \mathbf{u}_k^\top (\mathbf{x}_T - \mu)
$$

Effective computation

Analytical solution

$$\mathbf{x}_t = \mu + \frac{\sigma_t}{\sigma_T}(I - UU^\top)(\mathbf{x}_T - \mu) + \sum_{k=1}^{r} \sqrt{\frac{\lambda_k + \sigma_t^2}{\lambda_k + \sigma_T^2}} \mathbf{u}_k \mathbf{u}_k^\top (\mathbf{x}_T - \mu)$$

Additional second term is off-manifold term in case if U is rank deficient.

Score function

Instead of neural network $D_\theta(\mathbf{x}, \sigma)$ we have analytical solution

$$\begin{aligned} D(\mathbf{x}_t, \sigma_t) &= \mathbf{x}_t + \frac{1}{\sigma_t^2}(I - U\tilde{\Lambda}_{\sigma_t} U^\top)(\mu - \mathbf{x}_t) \\ &= \mu + \sum_{k=1}^{r} \frac{\lambda_k}{\sqrt{(\lambda_k + \sigma_t^2)(\lambda_k + \sigma_T^2)}} \mathbf{u}_k \mathbf{u}_k^\top (\mathbf{x}_T - \mu) \end{aligned}$$

Experiments Idea

Problem

We need to do many steps with $D_\theta(\mathbf{x}, \sigma)$ to get proper sample from ODE (1)

Empirical solution

If $p_{real}(\mathbf{x})$ is not normal we still can calculate mean μ and covariance Σ from data points. The Gaussian analytical solution provides a surprisingly good approximation to the early sampling trajectory. We skip several initial steps and start with

$$\mathbf{x}_t = \mu + \frac{\sigma_t}{\sigma_T}(I - UU^\top)(\mathbf{x}_T - \mu) + \sum_{k=1}^{r} c_k(\sigma_t)\mathbf{u}_k$$

and then continue with trained $D_\theta(\mathbf{x}_t, \sigma_t)$

Results of the experiment

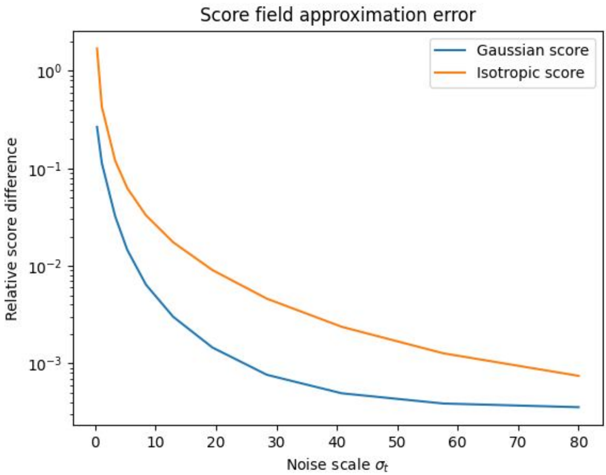


Figure 1: Approximation error of score learned by score neural network with analytical approximations

Results of the experiment

#(skipped steps)	FID
0	1.959
1	1.957
2	1.95
3	1.942
4	1.934
5	1.935
6	1.965
7	2.127
8	3.16
10	23.532
12	108.217

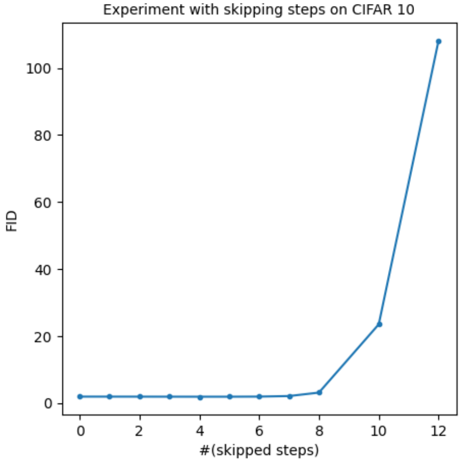


Figure 2: Image quality (FID score) of the method as a function of skipped steps on CIFAR10

Examples

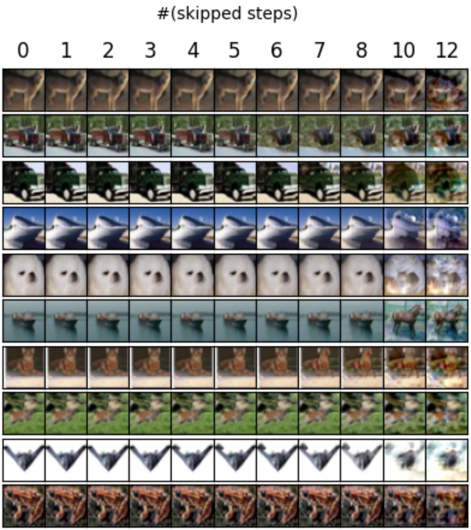


Figure 3: Sampled image as a function of skipped steps (from 18 steps)

Referenced paper

Wang, Binxu, and John J. Vastola
The Hidden Linear Structure in Score-Based Models and its Application
arXiv preprint arXiv:2311.10892 (2023).

Our Roles and Links

- Daniil and Kseniia – Code
- Bair, Arina, Nikita – Presentation and README
- Our GitHub
  `https://github.com/pkseniya/TheHiddenLinearStructureInScore-BasedModels`