

Interpreting and improving diffusion models from an optimization perspective

Chenyang Yuan (Joint work with Frank Permenter)

Blogpost/Code: chenyang.co/diffusion.html

Paper: arxiv.org/abs/2306.04848

Toyota Research Institute

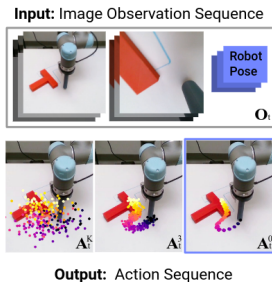
Friday 14th June, 2024

Introduction

Diffusion models achieve state-of-the-art results in multiple domains such as:



Image generation

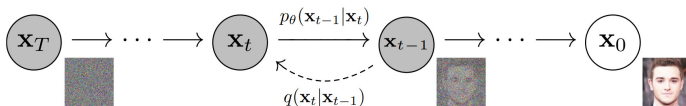


Trajectory planning

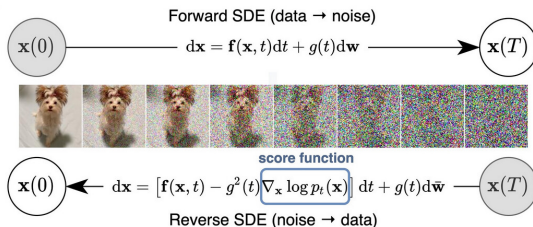
A powerful generative framework for sampling from multimodal distributions

Motivation

Diffusion models are motivated by probabilistic models



Reversal of stochastic process that adds noise to data (Ho et.al. 2020)



Sampling of data distribution using score function (Song et.al. 2021)

However, commonly used sampling procedures (e.g. DDIM) are deterministic

Motivation

Given commonly used diffusion training and sampling algorithms,

- Is there a deterministic model that motivates the same algorithms?
- Can we make reasonable assumptions on learned NN model to analyze performance of sampling algorithm?

Our optimization-based interpretation:

- Denoising approximates projection under manifold hypothesis
- Diffusion sampling finds projection to data manifold by minimizing distance via gradient descent

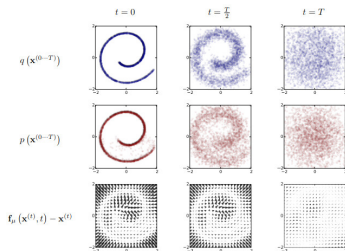
Training diffusion models

Denoising diffusion models estimate a **noise vector** $\epsilon \in \mathbb{R}^n$ from a given **noise level** $\sigma > 0$ and noisy input $x_\sigma \in \mathbb{R}^n$ such that for some x_0 in the **data manifold** \mathcal{K} ,

$$x_\sigma \approx x_0 + \sigma \epsilon$$

A **denoiser** $\epsilon_\theta : \mathbb{R}^n \times \mathbb{R}_+ \rightarrow \mathbb{R}^n$ is learned by minimizing

$$L(\theta) := \mathbf{E}_{x_0, \sigma, \epsilon} \|\epsilon_\theta(x_0 + \sigma \epsilon, \sigma) - \epsilon\|^2$$



*Note: to get expressions commonly used in literature, change of coordinates $z_t = \sqrt{\alpha_t} x_t$, where $\sigma_t^2 = (1 - \alpha_t)/\alpha_t$.

Visualization of training process

Distance and projection

The *distance function* $\text{dist}_{\mathcal{K}} : \mathbb{R}^n \rightarrow \mathbb{R}$ to a set $\mathcal{K} \subseteq \mathbb{R}^n$, is defined via

$$\text{dist}_{\mathcal{K}}(x) := \inf \{ \|x - x_0\| : x_0 \in \mathcal{K} \}$$

The *projection* of $x \in \mathbb{R}^n$, is the set of points that attain this distance

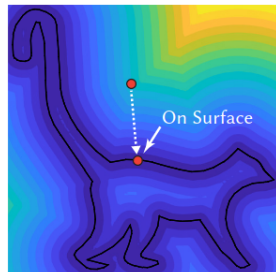
$$\text{proj}_{\mathcal{K}}(x) := \{x_0 \in \mathcal{K} : \text{dist}_{\mathcal{K}}(x) = \|x - x_0\|\}$$

Intuitively, $\text{proj}_{\mathcal{K}}(x) - x$ is the direction of steepest descent (i.e. neg. gradient) of $\text{dist}_{\mathcal{K}}(x)$.

Proposition

Suppose $\mathcal{K} \subseteq \mathbb{R}^n$ is closed and $x \notin \mathcal{K}$. If $\text{proj}_{\mathcal{K}}(x)$ is a singleton, then

$$\nabla \frac{1}{2} \text{dist}_{\mathcal{K}}(x)^2 = x - \text{proj}_{\mathcal{K}}(x)$$

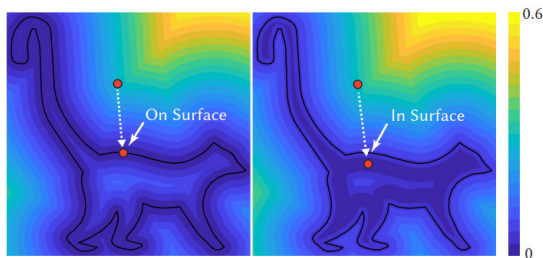


Smoothed distance and approximate projection

Distance function is not differentiable everywhere, $\nabla \text{dist}_{\mathcal{K}}(x)$ is not continuous, thus hard to learn!

Solution: σ -smoothed distance function

$$\text{dist}_{\mathcal{K}}(x, \sigma) := \text{softmin}_{x_0 \in \mathcal{K}}^{\sigma^2} \|x_0 - x\|^2 = -\sigma^2 \log \left(\sum_{x_0 \in \mathcal{K}} \exp \left(-\frac{\|x_0 - x\|^2}{2\sigma^2} \right) \right)$$



Smoothed distance function has continuous gradients

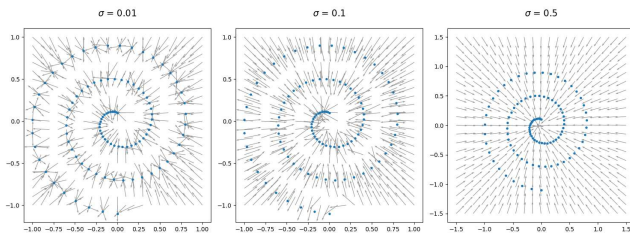
Ideal denoisers

The *ideal denoiser* is the minimizer of training loss, a function of data distribution \mathcal{K} and noise level σ

$$\epsilon^* := \arg \min_{\epsilon_\theta} \mathbf{E}_{x_0, \sigma, \epsilon} \|\epsilon_\theta(x_0 + \sigma\epsilon, \sigma) - \epsilon\|^2$$

For finite \mathcal{K} , there is a closed-form solution:

$$\epsilon^*(x_\sigma, \sigma) = \frac{\sum_{x_0 \in \mathcal{K}} (x_\sigma - x_0) \exp(-\|x_\sigma - x_0\|^2 / 2\sigma^2)}{\sigma \sum_{x_0 \in \mathcal{K}} \exp(-\|x_\sigma - x_0\|^2 / 2\sigma^2)}$$



Plot of direction of $\epsilon^*(x, \sigma)$ for different x and σ

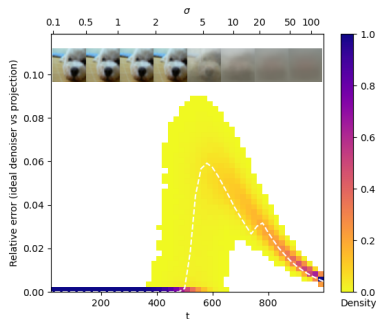
Ideal denoiser equivalent to gradient of smoothed distance

Theorem

For all $\sigma > 0$ and $x \in \mathbb{R}^n$, we have

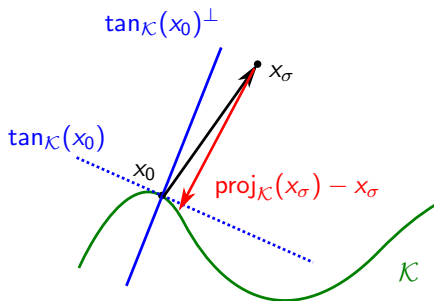
$$\frac{1}{2} \nabla_x \text{dist}_{\mathcal{K}}^2(x, \sigma) = \sigma \epsilon^*(x, \sigma).$$

- Does ideal denoiser approximate projection?
- We can compute relative error of learned denoiser v.s. ideal denoiser for CIFAR-10 dataset
- Plot error distribution for 10k different DDIM sampling trajectories



Denoising approximates projection: Low noise

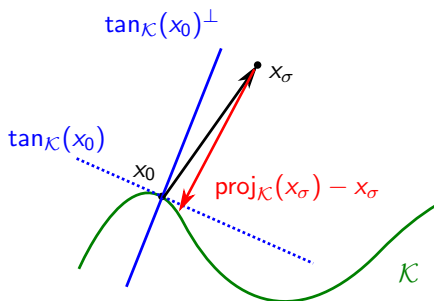
Manifold hypothesis: “real-world” datasets are (approximately) contained in low-dimensional manifolds \mathcal{K} of \mathbb{R}^n .



Given $x_\sigma = x_0 + \sigma\epsilon$, most of the added noise lies in $N_{\mathcal{K}}(x_0)$ with high probability, thus denoising approximates projection

Denoising approximates projection: Low noise

The *reach* of \mathcal{K} is the largest τ so that $\text{proj}_{\mathcal{K}}(x)$ is unique when $\text{dist}_{\mathcal{K}}(x) \leq \tau$



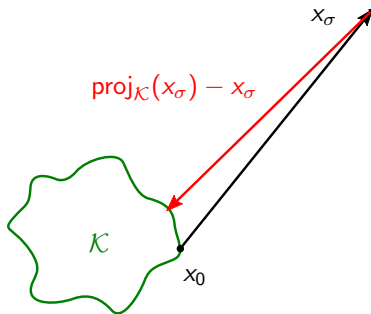
Theorem

Fix $\sigma > 0$ and suppose that $\text{reach}(\mathcal{K}) \gtrsim \sigma\sqrt{n}$. Given $x_0 \in \mathcal{K}$ and $\epsilon \sim \mathcal{N}(0, I)$, let $x_\sigma = x_0 + \sigma\epsilon$. With high probability, we have:

$$\|\text{proj}_{\mathcal{K}}(x_\sigma) - x_0\| \lesssim \sigma\sqrt{d}.$$

Denoising approximates projection: High noise

Diffusion models often add large levels of noise to x_0 in training, in order to start sampling from a Gaussian distribution



When σ is large, both denoising and projection point in the same direction towards \mathcal{K}

Denoising approximates projection

We claim that the denoiser learned from diffusion objective approximates projection with small relative error

- When σ small, manifold hypothesis tells us that most of noise added is orthogonal to data manifold
- When σ large, any weighted mean of data has small relative error
- Denoising with ideal denoiser is a σ -smoothing of $\text{proj}_{\mathcal{K}}(x)$ with small relative error

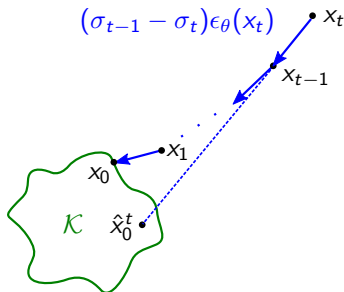
Next:

- Introduce relative error model
- Prove that diffusion sampling minimizes distance to data manifold under this error model

Sampling from diffusion models (Deterministic)

Given noisy x_σ and noise level σ , the learned denoiser $\epsilon_\theta(x_\sigma, \sigma)$ estimates

$$x_0 \approx \hat{x}_0(x_\sigma, \sigma) := x_\sigma - \sigma \epsilon_\theta(x_\sigma, \sigma).$$



Sampling algorithms (e.g. DDIM) construct a sequence $\hat{x}_0^t := \hat{x}_0(x_t, \sigma_t)$ of estimates from a sequence of points x_t using the update:

$$x_{t-1} = x_t + (\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t, \sigma_t)$$

Sampling from diffusion models (Probabilistic)

Deterministic (DDIM) update:

$$x_{t-1} = x_t + (\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t, \sigma_t)$$

Probabilistic (DDPM) update:

$$x_{t-1} = x_t + (\sigma_{t'} - \sigma_t)\epsilon_\theta(x_t, \sigma_t) + \eta w_t$$

Where $w_t \sim \mathcal{N}(0, I)$, $\sigma_{t'} = \sigma_{t-1}^2 / \sigma_t$ and $\eta = \sqrt{\sigma_{t-1}^2 - \sigma_{t'}^2}$
(Matches norm of update in expectation if $\mathbb{E} \|w_t\|^2 = \|\epsilon_\theta(x_t, \sigma_t)\|^2$)

Note: $\sigma_{t-1} = \sqrt{\sigma_t \sigma_{t'}}$, thus $\sigma_{t'} < \sigma_{t-1} < \sigma_t$.

These iterations look like gradient descent! But on which function?

Our error model

Let $f(x) := \frac{1}{2}\text{dist}_{\mathcal{K}}(x)^2$. Intuitively, $\nabla f(x) = x - \text{proj}_{\mathcal{K}}(x) \approx \text{dist}_{\mathcal{K}}(x)\epsilon_{\theta}(x)/\sqrt{n}$

Assumption (Projection with relative error)

There exists $\nu \geq 1$ and $\eta \geq 0$ such that if $\frac{1}{\nu}\text{dist}_{\mathcal{K}}(x) \leq \sqrt{n}\sigma_t \leq \nu\text{dist}_{\mathcal{K}}(x)$ and $\nabla f(x)$ exists, then $\|\sigma_t\epsilon_{\theta}(x, t) - \nabla f(x)\| \leq \eta\text{dist}_{\mathcal{K}}(x)$.

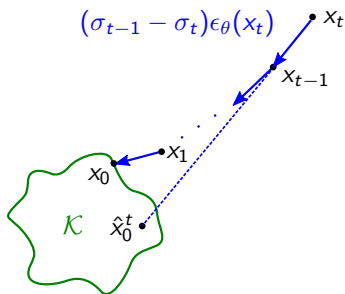
If $\sqrt{n}\sigma_t$ closely tracks $\text{dist}_{\mathcal{K}}(x)$, then $\sigma_t\epsilon_{\theta}(x, t)$ is approximately $\nabla f(x_t)$

- Relative error model where error depends on distance to \mathcal{K}
- Implications can be empirically tested on real datasets

DDIM is approximate gradient descent on f with stepsize $1 - \frac{\sigma_{t-1}}{\sigma_t}$, with $\nabla f(x_t)$ estimated by $\epsilon_{\theta}(x_t, \sigma_t)$

Intuitions on error model

If $\sqrt{n}\sigma_t$ closely tracks $\text{dist}_{\mathcal{K}}(x)$, then $\sigma_{t \in \theta}(x, t)$ is approximately $\nabla f(x_t)$



Projection at large noise levels is relatively inaccurate (tends to return data mean)

Projection at smaller noise levels is more accurate, but denoiser requires x_t to have noise level σ_t

Relative error assumption captures this intuition

Analysis under the error model

A schedule is $\{\sigma_t\}_{t=0}^N$ is (η, ν) -admissible when σ_t is decreased slow enough to maintain **relative error assumption**

- Log-linear (geometrically decreasing) schedules are (η, ν) -admissible
- $\sigma_{t-1} = (1 - \beta)\sigma_t$, with $\beta < C(\eta, \nu)$

We show convergence under the **relative error assumption**

Theorem (DDIM with relative error)

Let x_t denote the sequence generated by DDIM and suppose that the gradient of $f(x) := \frac{1}{2} \text{dist}_{\mathcal{K}}(x)^2$ exists for all x_t . Then for all t :

- $\frac{1}{\nu} \text{dist}_{\mathcal{K}}(x_t) \leq \sqrt{n} \sigma_t \leq \nu \text{dist}_{\mathcal{K}}(x_t)$,
- $\text{dist}_{\mathcal{K}}(x_N) \prod_{i=t}^N (1 - \beta_i(\eta + 1)) \leq \text{dist}_{\mathcal{K}}(x_{t-1}) \leq \text{dist}_{\mathcal{K}}(x_N) \prod_{i=t}^N (1 + \beta_i(\eta - 1))$.

Admissible schedule \implies Control of relative error $\implies \text{dist}_{\mathcal{K}}$ decreases

Improving sampling by gradient estimation

Our error model asserts that $\epsilon_\theta(x, \sigma) \approx \sqrt{n} \nabla \text{dist}_\mathcal{K}(x)$ when $\text{dist}_\mathcal{K}(x) \approx \sqrt{n} \sigma$.

Since $\nabla \text{dist}_\mathcal{K}(x)$ is *invariant* between x and $\text{proj}_\mathcal{K}(x)$, we aim to minimize estimation error $\sqrt{n} \nabla \text{dist}_\mathcal{K}(x) - \epsilon_\theta(x_t, \sigma_t)$, with the update

$$\bar{\epsilon}_t = \epsilon_\theta(x_{t+1}) + \gamma(\epsilon_\theta(x_t) - \epsilon_\theta(x_{t+1}))$$

Replaces $\epsilon_\theta(x_t, \sigma_t)$ in sampling algorithm

Corrects for error made in previous step using current estimate

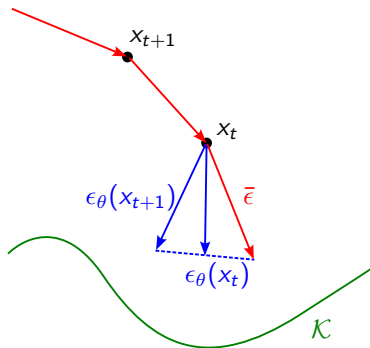


Illustration of our choice of $\bar{\epsilon}_t$

Empirically, $\gamma = 2$ achieves best results across many datasets and number of sampling steps

Improved sampling algorithm

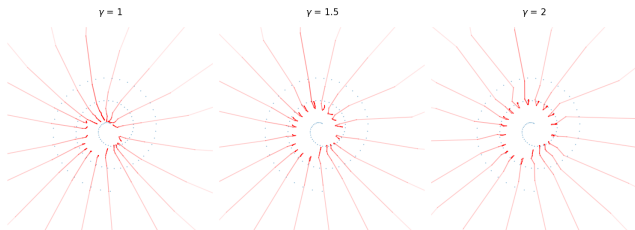
Given $(\sigma_N, \dots, \sigma_0)$, $x_N \sim \mathcal{N}(0, I)$ and ϵ_θ , to compute x_0 with N evaluations of ϵ_θ :

Algorithm 1 DDIM sampler

```
for  $t = N, \dots, 1$  do  
     $x_{t-1} \leftarrow x_t + (\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t, \sigma_t)$   
return  $x_0$ 
```

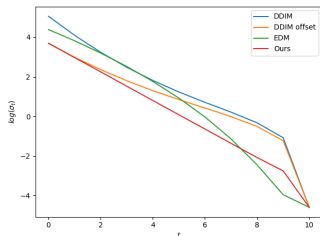
Algorithm 2 Our sampler

```
 $x_{N-1} \leftarrow x_N + (\sigma_{N-1} - \sigma_N)\epsilon_\theta(x_N, \sigma_N)$   
for  $t = N - 1, \dots, 1$  do  
     $\bar{\epsilon}_t \leftarrow 2\epsilon_\theta(x_t, \sigma_t) - \epsilon_\theta(x_{t+1}, \sigma_{t+1})$   
     $x_{t-1} \leftarrow x_t + (\sigma_{t-1} - \sigma_t)\bar{\epsilon}_t$   
return  $x_0$ 
```



Experiments on noise schedule

How should we choose σ_t ? Relative noise model suggests log-linear schedule



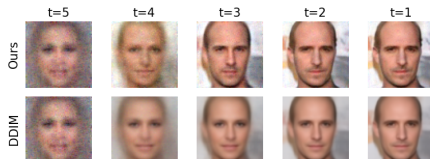
Plot of different choices of $\log(\sigma_t)$ for $N = 10$.

Schedule	CIFAR-10	CelebA
DDIM	16.86	18.08
DDIM Offset	14.18	15.38
EDM	20.85	16.72
Ours	13.25	13.55

FID scores of the DDIM sampler with different σ_t schedules on the CIFAR-10 model for $N = 10$ steps.

Sampler comparison experiments (Visual)

Visualizing \hat{x}_0^t throughout the denoising process:



A comparison of our sampler with DDIM on the CelebA dataset with $N = 5$ steps.

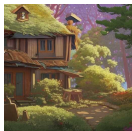
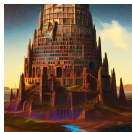
Sampler comparison experiments (FID)

Sampler	CIFAR-10 FID				CelebA FID			
	$N = 5$	$N = 10$	$N = 20$	$N = 50$	$N = 5$	$N = 10$	$N = 20$	$N = 50$
Ours	12.57	3.79	3.32	3.41	10.76	4.41	3.19	3.04
DDIM	47.20	16.86	8.28	4.81	32.21	18.08	11.81	7.39
PNDM	13.9	7.03	5.00	3.95	11.3	7.71	5.51	3.34
DPM		6.37	3.72	3.48		5.83	2.82	2.71
DEIS	18.43	7.12	4.53	3.78	25.07	6.95	3.41	2.95
UniPC	23.22	3.87						
A-DDIM		14.00	5.81*	4.04		15.62	9.22*	6.13

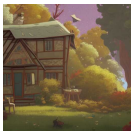
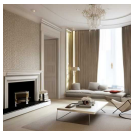
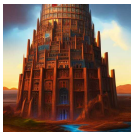
FID scores of our sampler compared to that of other samplers for pretrained CIFAR-10 and CelebA models with a discrete linear schedule. *Results for $N = 25$

Comparison on latent diffusion models

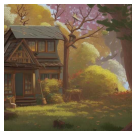
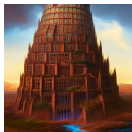
Ours
FID 13.77



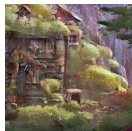
UniPC
15.59



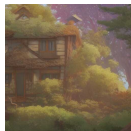
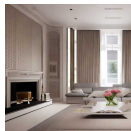
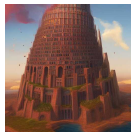
DPM++
15.43



PNDM
19.43



DDIM
14.06



Example outputs on text-to-image Stable Diffusion when limited to $N = 10$ function evaluations. FID scores for text-to-image generation on MS-COCO 30K.

Conclusion

Elementary deterministic framework for analyzing and generalizing diffusion models

- Simplified exposition of existing algorithms and methods
- New fast and simple-to-implement sampler designed with our interpretation

Framework for incorporating ideas from optimization into diffusion models

- Constraining diffusion models \leftrightarrow constrained optimization
- Use diffusion models in optimization problems (e.g. as a regularizer for compressed sensing)