Interpreting and improving diffusion models from an optimization perspective

Chenyang Yuan (Joint work with Frank Permenter)

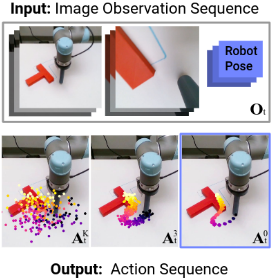
Toyota Research Institute

Tuesday 5th December, 2023

Introduction

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

Image generation

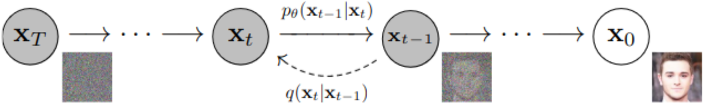


Trajectory planning

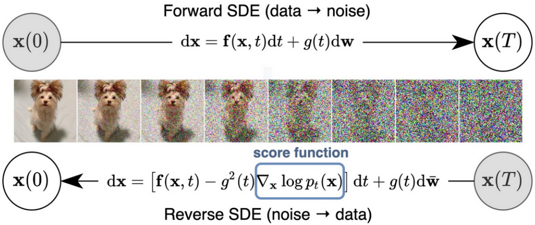
A powerful generative framework for sampling from multimodal distributions

Motivation

Diffusion models are motivated by probabilistic models


$\mathbf{x}_T$
$\mathbf{x}_t$
$p_\theta(\mathbf{x}_{t-1}|\mathbf{x}_t)$
$\mathbf{x}_{t-1}$
$q(\mathbf{x}_t|\mathbf{x}_{t-1})$
$\mathbf{x}_0$

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


Forward SDE (data → noise)
$\mathbf{x}(0)$
$\mathrm{d}\mathbf{x} = \mathbf{f}(\mathbf{x}, t)\mathrm{d}t + g(t)\mathrm{d}\mathbf{w}$
$\mathbf{x}(T)$
score function
$\mathbf{x}(0)$
$\mathrm{d}\mathbf{x} = \left[\mathbf{f}(\mathbf{x}, t) - g^2(t)\boxed{\nabla_{\mathbf{x}} \log p_t(\mathbf{x})}\right]\mathrm{d}t + g(t)\mathrm{d}\bar{\mathbf{w}}$
$\mathbf{x}(T)$
Reverse SDE (noise → data)

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

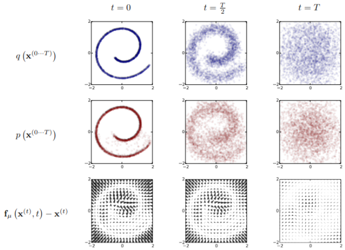
Training diffusion models

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

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



Visualization of training process

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

Distance and projection

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

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

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

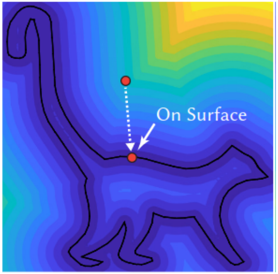
$$\mathrm{proj}_{\mathcal{K}}(x) := \{x_0 \in \mathcal{K} : \mathrm{dist}_{\mathcal{K}}(x) = \|x - x_0\|\}$$

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

Proposition

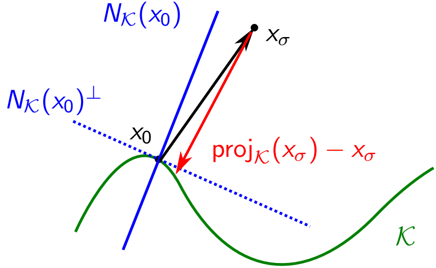
Suppose $\mathcal{K} \subseteq \mathbb{R}^n$ is closed and $x \notin \mathcal{K}$. If $\mathrm{proj}_{\mathcal{K}}(x)$ is a singleton, then

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



Denoising approximates projection: Low noise

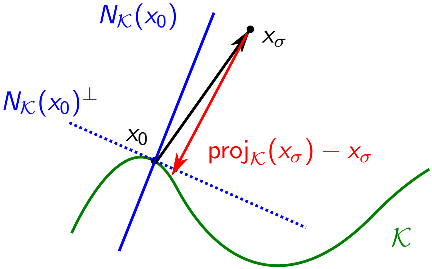
Manifold hypothesis: “real-world” datasets are (approximately) contained in low-dimensional manifolds $\mathcal{K}$ of of $\mathbb{R}^n$.


$N_{\mathcal{K}}(x_0)$
x_σ
$N_{\mathcal{K}}(x_0)^\perp$
x_0
$\text{proj}_{\mathcal{K}}(x_\sigma) - x_\sigma$
$\mathcal{K}$

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 $\mathrm{proj}_{\mathcal{K}}(x)$ is unique when $\mathrm{dist}_{\mathcal{K}}(x) \le \tau$



$N_{\mathcal{K}}(x_0)$
x_σ
$N_{\mathcal{K}}(x_0)^\perp$
x_0
$\mathrm{proj}_{\mathcal{K}}(x_\sigma) - x_\sigma$
$\mathcal{K}$

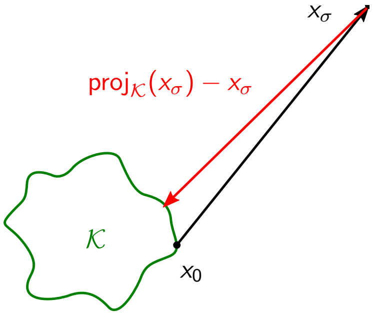
Theorem

Fix $\sigma > 0$ *and suppose that* $\mathrm{reach}(\mathcal{K}) \gtrsim \sigma\sqrt{n}$*. 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:*

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

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

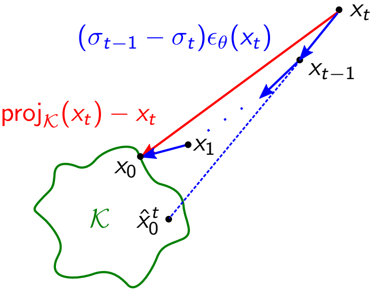


When σ is large, both denoising and projection point in the same direction towards $\mathcal{K}$

Sampling from diffusion models (Deterministic)

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

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



x_t
$(\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t)$
x_{t-1}
$\text{proj}_\mathcal{K}(x_t) - x_t$
x_1
x_0
$\mathcal{K}$
$\hat{x}_0^t$

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 $\mathbb{E}\left\|w_t\right\|^2 = \left\|\epsilon_\theta(x_t, \sigma_t)\right\|^2$)

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

Assumption (Projection with relative error)

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

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

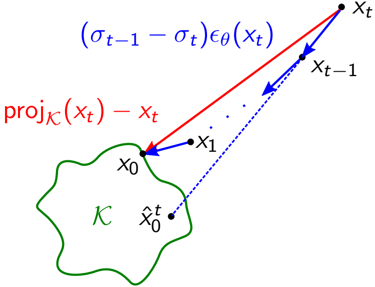
Relative error model where error depends on distance to $\mathcal{K}$

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 $\mathrm{dist}_{\mathcal{K}}(x)$, then $\sigma_t \epsilon_\theta(x, t)$ is approximately $\nabla f(x_t)$


x_t
$(\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t)$
x_{t-1}
$\mathrm{proj}_{\mathcal{K}}(x_t) - x_t$
x_1
x_0
$\mathcal{K}$
$\hat{x}_0^t$

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 $f(x) := \frac{1}{2}\mathrm{dist}_{\mathcal{K}}(x)^2$ exists for all x_t. Then for all t:

$$\frac{1}{\nu}\mathrm{dist}_{\mathcal{K}}(x_t) \leq \sqrt{n}\sigma_t \leq \nu \mathrm{dist}_{\mathcal{K}}(x_t),$$

$$\mathrm{dist}_{\mathcal{K}}(x_N)\prod_{i=t}^{N}(1-\beta_i(\eta+1)) \leq \mathrm{dist}_{\mathcal{K}}(x_{t-1}) \leq \mathrm{dist}_{\mathcal{K}}(x_N)\prod_{i=t}^{N}(1+\beta_i(\eta-1)).$$

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

Improving sampling by gradient estimation

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

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

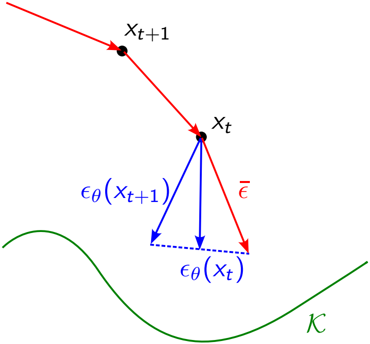


Illustration of our choice of $\bar{\epsilon}_t$

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

Improved sampling algorithm

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

Algorithm 1 DDIM sampler

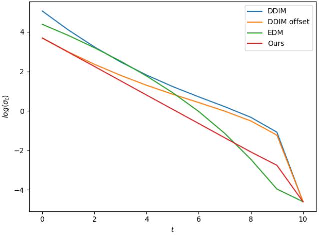
```
for $t = N, \ldots, 1$ do
    $x_{t-1} \leftarrow x_t + (\sigma_{t-1} - \sigma_t)\epsilon_\theta(x_t, \sigma_t)$
return $x_0$
```

Algorithm 2 Our sampler

```
$x_{N-1} \leftarrow x_N + (\sigma_{N-1} - \sigma_N)\epsilon_\theta(x_N, \sigma_N)$
for $t = N-1, \ldots, 1$ 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



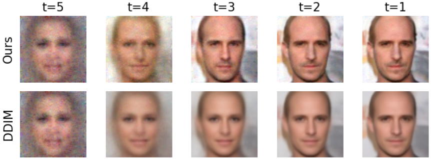
Plot of different choices of $\log(\sigma_t)$ for $N = 10$.

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.

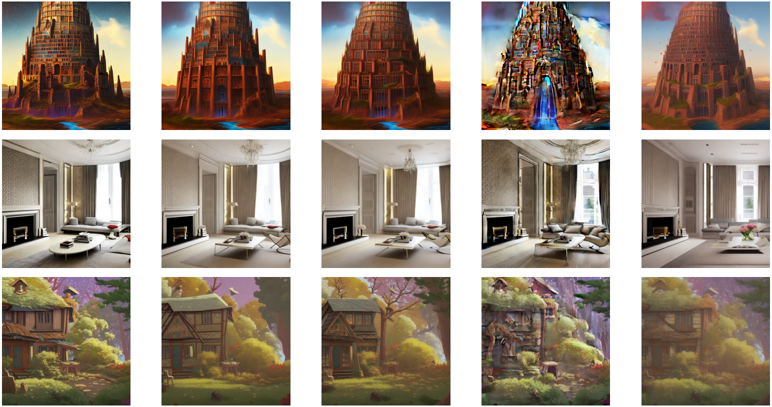
Sampler comparison experiments (FID)

	CIFAR-10 FID				CelebA FID			
Sampler	$N = 5$	$N = 10$	$N = 20$	$N = 50$	$N = 5$	$N = 10$	$N = 20$	$N = 50$
Ours	**12.53**	**3.85**	**3.39**	**3.43**	**10.73**	**4.30**	3.56	3.78
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	**UniPC**	**DPM++**	**PNDM**	**DDIM**
FID 13.77	15.59	15.43	19.43	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)