Bayesian Inverse Problem with Denoising Diffusion model priors

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Introduction

Generative modeling

We have a dataset $\mathcal{D}_N := \{X^1, \ldots, X^N\}$, where $X^i \in \mathbb{R}^{d_x}$.

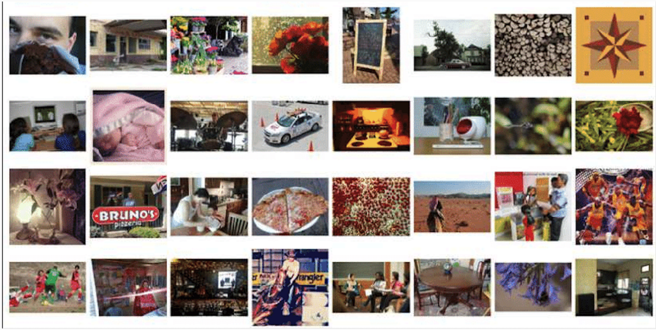

Figure 1: Samples from the `ImageNet` dataset.

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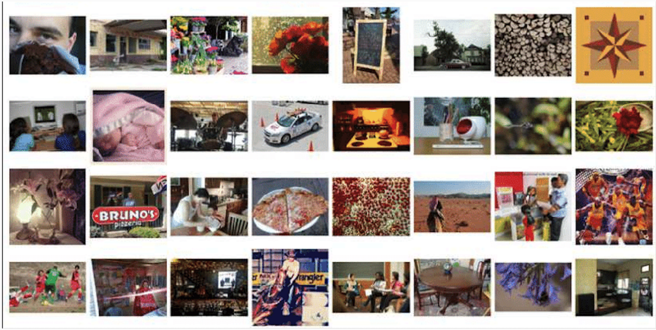

Figure 1: Samples from the `ImageNet` dataset.

Modeling assumption

$(X^1, \dots, X^N)$ are samples from some **unknown** distribution π_{data}

Generative modeling

① Approximate π_{data} with a parametric model.

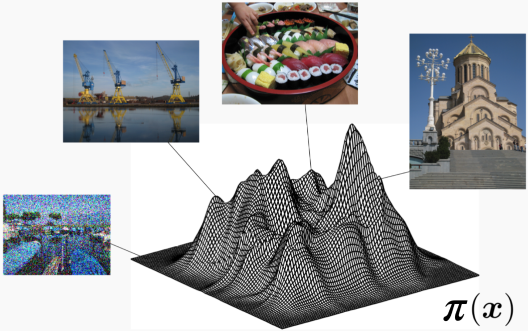

Figure 2: data distribution.

Bayesian inverse problems

② Sample reconstructions from the posterior distribution.

Figure 3: Reconstruction problems. Figure adapted from Lugmayr et al. (2022).

Generative modeling

① Approximate π_{data} with a parametric model p^{θ}.

Ackley et al. (1985); Kingma and Welling (2013); Goodfellow et al. (2014); Rezende and Mohamed (2015); Sohl-Dickstein et al. (2015); Ho et al. (2020); Song et al. (2021b)

Generative modeling

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1. Choose a suitable parametric form for p^{θ}.

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Generative modeling

① Approximate π_{data} with a parametric model p^θ.

1. Choose a suitable parametric form for p^θ.
2. Train p^θ to approximate π using the samples $(X^1, \ldots, X^N) \sim \pi$.

$$\mathcal{L}(\theta) = \sum_{i=1}^{N} -\log \mathsf{p}^\theta(X^i)\,.$$

$\rightsquigarrow$ Minimize $\mathcal{L}(\theta) \rightarrow$ find optimal parameter θ_*.

Ackley et al. (1985); Kingma and Welling (2013); Goodfellow et al. (2014); Rezende and Mohamed (2015); Sohl-Dickstein et al. (2015); Ho et al. (2020); Song et al. (2021b)

Posterior sampling

(2) Perform controlled generation using p^{θ_*}.

$\rightsquigarrow$ Target distribution: weight p^{θ_*} with a function $x \mapsto g(x)$

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⇝ Target distribution: weight p^{θ_*} with a function $x \mapsto g(x)$

$$\phi(\mathrm{d}x) = \frac{g(x)\mathsf{p}^{\theta_*}(\mathrm{d}x)}{\int g(z)\mathsf{p}^{\theta_*}(\mathrm{d}z)},$$

⇝ Posterior sampling: $g(x) = p(y|x)$.

⇝ Reinforcement learning: g is a reward function.

Denoising diffusion models

Introduction

- A denoising diffusion probabilistic model (DDPM) makes use of two Markov chains:
  1. a forward chain (process) that perturbs data to noise,
  2. a reverse chain (process) that converts noise back to data.
- The forward chain is typically hand-designed with the goal to transform the data distribution π_{data} into a (simple) reference distribution π_{ref} (e.g., standard Gaussian)
- The backward chain reverses the forward chain by learning transition kernels.
- New data points are generated by first sampling a random vector from the reference distribution, followed by ancestral sampling through the backward Markov chain.

Forward process

- Given a data distribution $x_0 \sim \pi_{\text{data}}(\mathrm{d}x_0) = q_0(\mathrm{d}x_0)$, the forward Markov chain generates a sequence of random variables $x_1, x_2 \ldots x_T$ with transition kernel $q_{t|t-1}(\mathrm{d}x_t \mid x_{t-1})$.
- The joint distribution of $x_1, x_2 \ldots x_T$ conditioned on x_0, denoted as $q_{0:T}(\mathrm{d}(x_1, \ldots, x_T) \mid x_0)$, may be written as

$$q_{0:T}(\mathrm{d}(x_1, \ldots, x_T) \mid x_0) = \prod_{t=1}^{T} q_{t|t-1}(\mathrm{d}x_t \mid x_{t-1}).$$

- In DDPMs, we handcraft the transition kernel $q_{t|t-1}(\mathrm{d}x_t \mid x_{t-1})$ to incrementally transform the data distribution $q_0(\mathrm{d}x_0)$ into a tractable reference distribution.
  - Typical design: Gaussian perturbation

$$q_{t|t-1}(x_t \mid x_{t-1}) = \mathcal{N}\left(x_t; \sqrt{1-\beta_t}\, x_{t-1}, \beta_t \mathbf{I}\right),$$

    where $\beta_t \in (0, 1)$ is a hyperparameter chosen ahead of model training.

Forward process

- Gaussian transition kernel allows us to obtain the analytical form of $q_{t|0}(x_t \mid x_0)$ for all $t \in \{0, 1, \cdots, T\}$. Setting $\alpha_t := 1 - \beta_t$ and $\bar{\alpha}_t := \prod_{s=0}^{t} \alpha_s$, we have

$$q_{t|0}(x_t \mid x_0) = \mathcal{N}\left(x_t; \sqrt{\bar{\alpha}_t} x_0, (1 - \bar{\alpha}_t)\mathbf{I}\right).$$

- Given x_0, we can easily obtain a sample of x_t by sampling a Gaussian vector $\epsilon_t \sim \mathcal{N}(0, \mathrm{I})$ and applying the transformation

$$x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1 - \bar{\alpha}_t} \boldsymbol{\epsilon}_t.$$

- When $\bar{\alpha}_T \approx 0, x_T$ is almost Gaussian in distribution,

$$q_T(x_T) := \int q_{T|0}(x_T \mid x_0)\, q_0(x_0)\, \mathrm{d}x_0 \approx \mathcal{N}(x_T; \mathbf{0}, \mathbf{I}).$$

Backward process

- For generating new data samples, DDPMs start by sampling the reference distribution and then gradually remove noise by running a learnable Markov chain backward in time.
- The reverse Markov chain is parameterized by a reference distribution $\pi_{\text{ref}}(x_T) = \mathcal{N}(x_T; \mathbf{0}, \mathrm{I})$ and a learnable transition kernel

$$p^{\theta}_{t-1|t}(x_{t-1} \mid x_t) = \mathcal{N}\left(x_{t-1}; \mu^{\theta}_t(x_t), \Sigma^{\theta}_t(x_t)\right)$$

  where θ denotes model parameters, and the mean $\mu^{\theta}_t(x_t)$ and variance $\Sigma^{\theta}_t(x_t)$ are parameterized by deep neural networks.
- Data generation
  - Sample $x_T \sim \pi_{\text{ref}}(\cdot)$,
  - iteratively sample $x_{t-1} \sim p^{\theta}_{t-1|t}(\cdot \mid x_t)$ until $t = 1$.

Diffusion model principles

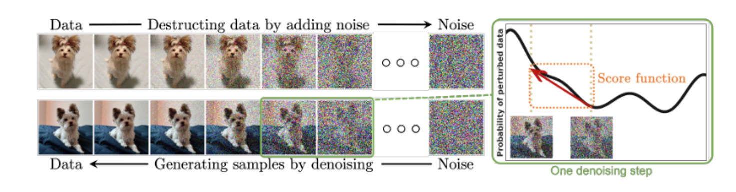

Figure 4: Diffusion models smoothly perturb data by adding noise, then reverse this process to generate new data from noise.

Variational Inference

- Objective: Adjust the parameter θ so that the joint distribution of the reverse Markov chain

$$p_{0:T}^{\theta}\left(x_0, x_1, \cdots, x_T\right) = p_{\mathrm{ref}}(x_T) \prod_{t=1}^{T} p_{t-1|t}^{\theta}(x_{t-1} \mid x_t)$$

matches

$$q_{0:T}\left(x_0, x_1, \cdots, x_T\right) := q_0\left(x_0\right) \prod_{t=1}^{T} q_{t|t-1}\left(x_t \mid x_{t-1}\right).$$

- Training is performed by maximizing a variational bound:

$$\mathbb{E}_{q_0}\left[-\log p^{\theta}\left(x_0\right)\right] \leq \mathbb{E}_{q_{0:T}}\left[-\log \frac{p_{0:T}^{\theta}\left(x_{0:T}\right)}{q_{1:T|0}\left(x_{1:T} \mid x_0\right)}\right]$$

$$= \mathbb{E}_{q_{0:T}}\left[-\log p_T\left(x_T\right) - \sum_{t\geq 1} \log \frac{p_{t-1|t}^{\theta}\left(x_{t-1} \mid x_t\right)}{q_{t|t-1}\left(x_t | x_{t-1}\right)}\right] =: L^{\theta}$$

Variational inference with variance reduction

- L^θ might be rewritten using the backward representation of the forward noising process

$$q_{1:T|0}(x_{1:T}|x_0) = \prod_{t=1}^{T} q_{t|t-1}(x_t|x_{t-1})$$
$$= q_{T|0}(x_T|x_0) \prod_{t=2}^{T} q_{t-1|t}(x_{t-1}|x_t, x_0)$$

- With this backward decomposition, L^θ writes

$$L^\theta = \mathbb{E}_{q_{0:T}}\left[- \log \frac{p_T(x_T)}{q_{T|0}(x_T \mid x_0)} - \sum_{t=2}^{T} \log \frac{p^\theta_{t-1|t}(x_{t-1} \mid x_t)}{q_{t-1|t,0}(x_{t-1} \mid x_t, x_0)} - \log p^\theta_{0|1}(x_0 \mid x_1)\right]$$

$$= \mathbb{E}_{q_{0:T}}\left[D_{\mathrm{KL}}\left(q_{T|0}(\cdot \mid x_0) \| p_T(\cdot)\right) + \sum_{t=2}^{T} D_{\mathrm{KL}}\left(q_{t-1|t,0}(\cdot \mid x_t, x_0) \| p^\theta_{t-1|t}(\cdot \mid x_t)\right) - \log p^\theta_{0|1}(x_0 \mid x_1)\right]$$

Variational inference with variance reduction

- forward posteriors are tractable when conditioned on x_0 :

$$q_{t-1|t,0}\left(x_{t-1} \mid x_t, x_0\right) = \mathcal{N}\left(x_{t-1}; \tilde{\boldsymbol{\mu}}_t\left(x_t, x_0\right), \tilde{\beta}_t \mathbf{I}\right)$$

$$\text{where} \quad \tilde{\boldsymbol{\mu}}_t\left(x_t, x_0\right) := \frac{\sqrt{\bar{\alpha}_{t-1}}\beta_t}{1-\bar{\alpha}_t} x_0 + \frac{\sqrt{\alpha_t}\left(1-\bar{\alpha}_{t-1}\right)}{1-\bar{\alpha}_t} x_t$$

$$\text{and} \quad \tilde{\beta}_t := \frac{1-\bar{\alpha}_{t-1}}{1-\bar{\alpha}_t}\beta_t$$

- KL divergences are comparisons between Gaussian distributions with closed form expressions: taking $\Sigma_t^\theta(x_t) = \tilde{\beta}_t \mathrm{I}$,

$$D_{\mathrm{KL}}\left(q_{t-1|t,0}\left(\cdot \mid x_t, x_0\right) \| p^\theta_{t-1|t}\left(\cdot \mid x_t\right)\right) = \frac{1}{2\tilde{\beta}_t}\|\tilde{\boldsymbol{\mu}}_t(x_t, x_0) - \mu_t^\theta(x_t)\|^2 .$$

Variational inference with variance reduction

- Setting

$$\mu_t^\theta(x_t) = \tilde{\mu}_t(x_t, \hat{x}_{0|t}^\theta(x_t)),$$

we get

$$D_{\mathrm{KL}}\left(q_{t-1|t,0}\left(\cdot \mid x_t, x_0\right) \| p_{t-1|t}^\theta\left(\cdot \mid x_t\right)\right) = w_t \|x_0 - \hat{x}_{0|t}^\theta(x_t)\|^2 .$$

with $w_t = \bar{\alpha}_{t-1}\beta_t/(1-\bar{\alpha}_{t-1})(1-\bar{\alpha}_t)$.

- Hence, criterion L^θ rewrites

$$L^\theta = \sum_{t=2}^{T} w_t \mathbb{E}_{q_0 \otimes \mathcal{N}(0,\mathrm{I})}[\|x_0 - \hat{x}_{0|t}^\theta(\sqrt{\bar{\alpha}_t}x_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon})\|^2]$$

which amount to compute $\hat{x}_{0|t}^\theta(x_t)$ as a predictor of the initial state x_0 from the current state x_t.

- This criterion is the denoising score matching.

Noise prediction

- Using that $x_t = \sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t$, we have

$$x_0 = \frac{1}{\sqrt{\bar{\alpha}_t}}(x_t - \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon}_t)$$

- Choosing $\hat{x}^{\theta}_{0|t}(x_t) = (1/\sqrt{\bar{\alpha}_t})(x_t - \sqrt{1-\bar{\alpha}_t}\hat{\boldsymbol{\epsilon}}^{\theta}_{0|t}(x_t))$, the criterion L^{θ} may be equivalently expressed as

$$L^{\theta} = \sum_{t=2}^{T} \tilde{w}_t \mathbb{E}_{q_0 \otimes \mathcal{N}(0,\mathrm{I})}[\|\boldsymbol{\epsilon} - \hat{\boldsymbol{\epsilon}}^{\theta}_{0|t}(\sqrt{\bar{\alpha}_t} x_0 + \sqrt{1-\bar{\alpha}_t}\boldsymbol{\epsilon})\|^2]$$

where

$$\tilde{w}_t = \frac{\beta_t}{\alpha_t(1-\bar{\alpha}_{t-1})}$$

A continuous-time perspective

Ornstein-Uhlenbeck Noising process

- Consider a diffusion process $\{X_t\}_{t=0}^{T}$ that starts from the data distribution $q_0(\mathrm{d}x) \equiv \pi_{\mathsf{data}}(\mathrm{d}x)$ at time $t = 0$. The notation $q_t(\mathrm{d}x)$ refers to the marginal distribution of the diffusion at time $0 \leq t \leq T$.
- Assume furthermore that at time $t = T$, the marginal distribution is (very close to) a reference distribution $q_T(\mathrm{d}x) = \pi_{\mathsf{ref}}(\mathrm{d}x)$ that is straightforward to sample from, e.g. $\mathcal{N}(0, \mathrm{I})$.
- This diffusion process is the noising process. It is often chosen as an Ornstein-Uhlenbeck (OU) diffusion,

$$\mathrm{d}X_t = -\frac{1}{2} X_t \mathrm{d}t + \mathrm{d}W_t$$

OU noising process

- OU diffusion is reversible w.r.t. $\pi_{\text{ref}} = \mathcal{N}(0, \mathrm{I})$: the conditional distribution of $X_{t+s} \mid X_t = x_t$ is $\mathcal{N}(\alpha_s x_t, \sigma_s^2 \mathrm{I})$, with

$$\alpha_s = \sqrt{1 - \sigma_s^2} \quad \sigma_s^2 = 1 - \mathrm{e}^{-s}$$

- Denote

$$F(s, x, y) \propto \exp\left\{-\frac{(y - \alpha_s x)^2}{2\sigma_s^2}\right\}.$$

the forward transition from x to y in " s " amount of time.

Reverse diffusion I (informal)

- the DDPM strategy consists in sampling from the Gaussian reference measure π_{ref} at time $t = T$ and simulate the OU process backward in time.
- In other words, one would like to simulate from the reverse process $\overleftarrow{X}_t$ defined as

$$\overleftarrow{X}_s = X_{T-s}$$

- The reverse process is distributed as $\overleftarrow{X}_0 \sim \pi_{\text{ref}}$ at time $t = 0$ and, crucially, we have that $\overleftarrow{X}_T \sim \pi_{\text{data}}$.
- The reverse diffusion follows the dynamics (Hausmann, Pardoux, 1986; Millet, Nualart, Sanz, 1989)

$$d\overleftarrow{X}_t = +\frac{1}{2}\overleftarrow{X}_t dt + \nabla \log q_{T-t}\left(\overleftarrow{X}_t\right) \mathrm{d}t + \mathrm{d}B_t$$

where B is another Wiener process [the notation B emphasizes that there is no link between this Wiener process and the one used to simulate the forward process].

Reverse diffusion II (informal)

- To simulate the reverse diffusion, one needs to be able to estimate the score $\nabla \log q_{T-t}(x)$.
- In practice, the score is unknown and need to be approximated

$$s_t^\theta(x) \approx \nabla_x \log q_t(x)$$

which is often parameterized by a neural network.

- Since

$$\log q_t(x) = \log \int F(t, x_0, x) \, \pi_{\mathsf{data}} \, (\mathrm{d}x_0)$$

the analytical expression of $F(t, x_0, x)$ gives that (Tweedie formula)

$$\nabla_x \log q_t(x) = -\frac{x - \alpha_t \widehat{x}_0(x,t)}{\sigma_t^2}$$

where $\widehat{x}_0(x,t) = \mathbb{E}\left[X_0 | X_t = x\right]$ is a denoising estimate of x_0 given a noisy estimate $X_t = x$ at time t

Estimation of the score

- To estimate the score, one only needs to train a denoising function $\widehat{x}^{\theta}_{0|t}(x)$.
- It is a simple regression problem: take pairs (X_0, X_t) that can be generated as

$$X_0 \sim \pi_{\text{data}} \quad \text{and} \quad X_t = \alpha_t X_0 + \sigma_t Z_t$$

  with $Z_t \sim \mathcal{N}(0, \mathrm{I})$ and minimize the Mean Squared Error (MSE) loss, i.e.

$$\mathbb{E}_{q_{0,t}}\left[\left\|X_0 - \hat{x}^{\theta}_{0|t}(X_t)\right\|^2\right]$$

  with stochastic gradient descent or any other stochastic optimization procedure.
- The score is then defined as

$$s^{\theta}_t(x) = -\frac{x - \alpha_t \widehat{x}^{\theta}_t(x)}{\sigma_t^2}$$

Time reversal formula for a diffusion process

General time reversal formulas for diffusion processes are well known since the 80 's. Consider a diffusion process Y in $\mathbb{R}^n$ satisfying

$$dY_t = b_t\,(Y_t)\,dt + \sigma_t\,(Y_t)\,dB_t, \quad 0 \le t \le T,$$

with B a Brownian motion, b a drift vector field and σ a matrix field associated to the diffusion field a $:= \sigma\sigma^\top$

Assuming that the law of Y_t is absolutely continuous at each time t, under appropriate assumptions, the time-reversed process Y^* is again a diffusion process with diffusion matrix field $\mathrm{a}_t^* = \mathrm{a}_{T-t}$ and drift field

$$b_t^*(y) = -b_{T-t}(y) + \nabla \cdot (\mu_{T-t}\mathrm{a}_{T-t})\,(y)/\mu_{T-t}(y),$$

where μ_t is the density of the law of Y_t with respect to Lebesgue measure.

This is not a straightforward result because a reversed semimartingale might not be a semimartingale !.

Time reversal formula for a diffusion process

For the identity

$$b_t^*(y) = -b_{T-t}(y) + \nabla \cdot \left(\mu_{T-t} \mathrm{a}_{T-t}\right)(y)/\mu_{T-t}(y),$$

to hold, it is assumed in that b is locally Lipschitz and that either a is bounded away from zero or that the derivative ∇a in the sense of distribution is controlled locally.

Haussmann and Pardoux take a PDE approach; Millet, Nualart and Sanz rely on stochastic calculus of variations.

The existence of an absolutely continuous density follows from a Hörmander type condition (PDE formulation in Haussman et al. and consequence of Malliavin calculus in Millet et al.).

Time reversal formula for a diffusion process

Föllmer's approach significantly departs from these strategies. Under the simplifying hypothesis that a is the identity matrix, the law P of Y has a finite entropy

$$H(P \mid R) < \infty$$

with respect to the law R of a Brownian motion with some given initial probability distribution.

In particular, the drift field b of P satisfies $\int_{[0,T]\times\mathbb{R}^n} |b_t(y)|^2 \mu_t(y) dt dy < \infty$ and might be singular, rather than locally Lipschitz.

As a consequence of this finite entropy assumption, Föllmer proves the time reversal formula

$$b_t^*(y) = -b_{T-t}(y) + \nabla \log \mu_{T-t}(y)$$

(recall a = Id) where the derivative is in the sense of distributions, without invoking any already known result about the regularity of μ.

Summary

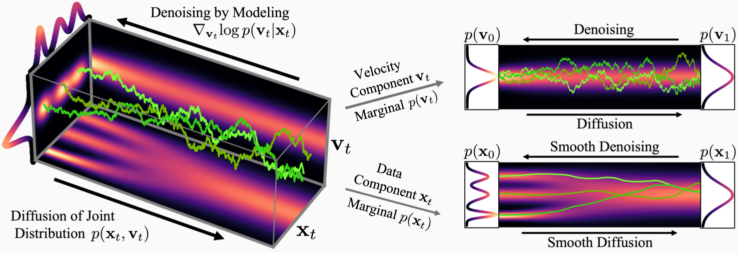

Figure 5: From Dockhorn et al. (2022)

Feyman-Kac representation

Context

Bayesian linear inverse problem:

$$Y = AX + \sigma_y Z, \quad \text{where} \quad Z \sim \mathcal{N}(\mathbf{0}_{d_x}, \mathrm{I}_{d_x}), \quad X \sim p_0, \quad \sigma_y \geq 0\,.$$

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Objective: Sample the distribution of X given a realisation y of Y.

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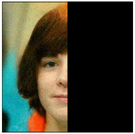
Sample from p_0

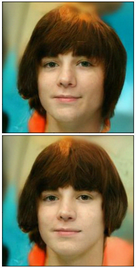
$\xrightarrow{AX+\sigma_y Z}$

Observation y



$\longrightarrow$

Posterior samples



Feynman-Kac representation

We focus on the specific case where the prior p_0 is the marginal w.r.t. x_0 of Denoising Diffusion Model. The posterior is

$$p_0^y(\mathrm{d}x_0) = \frac{1}{\mathcal{Z}^y} \int g_0^y(x_0) \prod_{k=0}^{n-1} p_{k|k+1}(\mathrm{d}x_k|x_{k+1})\, p_n(\mathrm{d}x_n)\,.$$

- The posterior can be interpreted as the marginal of a (time-reversed) Feynman–Kac (FK) model with non-trivial potential only at $k = 0$!
- In this work, we twist, without modifying the law of the FK model, the backward transitions $p_{k|k+1}$ by potentials depending on the observation y; see *e.g.* for a similar idea for rare event simulation (see, *e.g.*, Cérou et al., 2012).

"Forward" smoothing decomposition

- Define, for all $k \in [\![0, n]\!]$, the backward functions

$$\beta^y_{0|k}(x_k) := \int g^y_0(x_0)\, p_{0|k}(\mathrm{d}x_0|x_k)$$

- The backward functions satisfy the recursion:

$$\beta^y_{0|k+1}(x_{k+1}) = \int \beta^y_{0|k}(x_k)\, p_{k|k+1}(\mathrm{d}x_k|x_{k+1})\,.$$

- Define the forward smoothing kernels (FSK) for $k \in [\![0, n-1]\!]$

$$p^y_{k|k+1}(\mathrm{d}x_k|x_{k+1}) := \frac{\beta^y_{0|k}(x_k)}{\beta^y_{0|k+1}(x_{k+1})}\, p_{k|k+1}(\mathrm{d}x_k|x_{k+1})\,,$$

$$(= \mathrm{Law}(X_k \mid Y = y, X_{k+1} = x_{k+1}))\,.$$

"Forward" smoothing decomposition

The posterior distribution can be written in terms of forward smoothing kernels

$$p_0^y(\mathrm{d}x_0) = \int p_n^y(\mathrm{d}x_n) \prod_{k=0}^{n-1} p_{k|k+1}^y(\mathrm{d}x_k|x_{k+1}) \,.$$

where

$$p_n^y(\mathrm{d}x_n) = \frac{\beta_{0|n}^y(x_n) p_n(\mathrm{d}x_n)}{\mathcal{Z}^y}$$

- Most of the recent works to sample from p_0^y use the forward smoothing decomposition with different approximation of the intractable forward smoothing kernels. Chung et al. (2023); Song et al. (2023); Zhang et al. (2023); Boys et al. (2023); Trippe et al. (2023); Wu et al. (2023).

DDPM approximation

The DDPM is based on the assumption the forward smoothing decomposition is a good approximation the time reversal of the forward Markov chain initialized at p_0^y, i.e.

$$p_0^y(\mathrm{d}x_0) \prod_{k=1}^{n} q_{k|k-1}(\mathrm{d}x_k|x_{k-1}) \approx p_n^y(\mathrm{d}x_n) \prod_{k=0}^{n-1} p_{k|k+1}^y(\mathrm{d}x_k|x_{k+1}) \,,$$

which suggests the following approximation

$$p_{k|k+1}^y(\mathrm{d}x_k|x_{k+1}) \approx \int q_{k|0,k+1}(\mathrm{d}x_k|x_0, x_{k+1}) p_{0|k+1}^y(\mathrm{d}x_0|x_{k+1})$$

where

$$p_{0|k+1}^y(\mathrm{d}x_0|x_{k+1}) \propto p_0^y(\mathrm{d}x_0) q_{k+1|0}(x_{k+1}|x_0)$$

DDPM approximation

(Ho et al., 2020; Song et al., 2021a) suggested to use the DDPM approximation of the backward kernel is :

$$p^y_{k|k+1}(\mathrm{d}x_k|x_{k+1}) = q_{k|0,k+1}(\mathrm{d}x_k|\mathbb{E}[X_0|X_{k+1} = x_{k+1}, Y = y], x_{k+1})$$

where

$$\mathbb{E}[X_0|X_{k+1}, Y = y] := \int x_0 \, p^y_{0|k+1}(\mathrm{d}x_0|X_{k+1}) \, .$$

Conditional score

By Tweedie's formula,

$$\mathbb{E}\big[X_0|X_k, Y = y\big] = \frac{X_k + (1-\alpha_k)\nabla_{x_k}\log p_k^y(X_k)}{\sqrt{\alpha_k}}\,,$$

where

$$\begin{aligned} p_k^y(x_k) &:= \int p_0^y(\mathrm{d}x_0) q_{k|0}(x_k|x_0) \\ &\propto \int g_0^y(x_0) p_0(\mathrm{d}x_0) q_{k|0}(x_k|x_0) \\ &\propto \int g_0^y(x_0) p_{0|k}(\mathrm{d}x_0|x_k)\, p_k(x_k)\,. \end{aligned}$$

Hence,

$$\nabla_{x_k}\log p_k^y(x_k) = \nabla_{x_k}\log \beta_{0|k}^y(x_k) + \nabla_{x_k}\log p_k(x_k)\,.$$

Diffusion posterior sampling I

$$\nabla_{x_k} \log p_k^y(x_k) = \nabla_{x_k} \log \beta_{0|k}^y(x_k) + \nabla_{x_k} \log p_k(x_k)\,,$$

- A pre-trained score network (for $\nabla_{x_k} \log p_k(x_k)$) is available.
- But the gradient of the log backward function is intractable in practice.

Using the pre-trained approximation $\hat{x}_{0|k}(X_k)$ of $\mathbb{E}[X_0|X_k]$, Chung et al. (2023) proposed the following approximation,

$$\nabla_{x_k} \log \beta_{0|k}^y(x_k) \approx \nabla_{x_k} \log g_0^y(\hat{x}_{0|k}(x_k))\,.$$

They then sample approximately from the FSK in the following way; given X_k^y

- First sample $X_{k-1} \sim p_{k-1|k}(\cdot|X_k^y)$
- Then set $X_{k-1}^y = X_{k-1} + \gamma_k \nabla_{x_k} \log g_0^y(\hat{x}_{0|k}(X_k^y))$
- γ_k is in practice a highly sensitive parameter, crucial for good performance.

Diffusion posterior sampling II

- The DPS approximation by Chung et al. (2023) boils down to assuming that $p_{0|k}(\mathrm{d}x_0|x_k) \approx \delta_{\hat{x}_{0|k}(x_k)}(\mathrm{d}x_0)$.
- This is a very crude approximation that becomes accurate only as $k \to 0$.

Song et al. (2023) consider the sample sampling scheme but propose instead the following Gaussian approximation

$$p_{0|k}(\mathrm{d}x_0|x_k) \approx \mathcal{N}(\mathrm{d}x_0; \hat{x}_{0|k}(x_k), r_k^2 \,\mathrm{I}_{d_x}), \quad r_k^2 = \frac{\sigma_k^2}{1+\sigma_k^2}\,,$$

in which case, we obtain the following approximation

$$\beta^y_{0|k}(x_k) \approx \mathcal{N}(y; A\hat{x}_{0|k}(x_k), r_k^2 A A^\intercal + \sigma_y^2 \,\mathrm{I}_{d_y})\,.$$

- The Gaussian approximation above becomes exact in the case where $p_0 = \mathcal{N}(\mathbf{0}_{d_x}, \mathrm{I}_{d_x})$ and *variance exploding* is used.
- Still, this is not a realistic approximation in the more general case.

Tweedie Moment Projected diffusion

Boys et al. (2023) instead consider a Gaussian approximation $\hat{p}_{0|k}(\cdot|x_k)$ of $p_{0|k}(\cdot|x_k)$:

$$\hat{p}_{0|k}(\cdot|x_k) := \underset{\mu,\Sigma}{\operatorname{argmin}} \mathsf{KL}(p_{0|k}(\cdot|x_k) \parallel \mathcal{N}(\mu, \Sigma)) .$$

and

$$\hat{p}_{0|k}(\cdot|x_k) = \mathcal{N}\big(\mathbb{E}[X_0|X_k = x_k], \mathbb{C}\text{ov}(X_0|X_k = x_k)\big) ,$$

where the expectation and covariance are under $p_{0|k}(\cdot|x_k)$. Under the same assumption as previously (backward=forward), it can be shown that

$$\mathbb{C}\text{ov}(X_0|X_k) = \frac{1-\alpha_k}{\sqrt{\alpha_k}} \nabla_{x_k} \mathbb{E}[X_0|X_k]$$

which may be approximated by plugging in $\hat{x}_{0|k}(X_k)$ to approximate $\nabla_{x_k} \mathbb{E}[X_0|X_k]$.

- The resulting covariance approximation is not symmetric nor positive definite.
- Extremely expensive to compute. In practice further crude approximations are introduced.

Monte Carlo guided diffusion

General Feynman–Kac model

Introduce intermediate positive potentials $(g_k^y)_{k=0}^n$, each being a function on $\mathbb{R}^{d_x}$, and write

$$p_0^y(\mathrm{d}x_0) = \frac{1}{\mathcal{Z}^y} \int g_n^y(x_n)\, p_n(\mathrm{d}x_n) \times \prod_{k=0}^{n-1} \frac{g_k^y(x_k)}{g_{k+1}^y(x_{k+1})}\, p_{k|k+1}(\mathrm{d}x_k|x_{k+1})\,.$$

- Because the $g_n^y(x_n) \prod_{k=0}^{n-1} \frac{g_k^y(x_k)}{g_{k+1}^y(x_{k+1})} = g_0^y(x_0)$, the FK is not modified - the potentials are used to render the sampling easier.
- This allows the posterior of interest to be expressed as the time-zero marginal of a Feynman-Kac model with
  - initial law p_n,
  - Markov transition kernels $(p_{k|k+1})_{k=0}^{n-1}$
  - Potentials g_n^y and $(x_k, x_{k+1}) \mapsto g_k^y(x_k)/g_{k+1}^y(x_{k+1})$.

Posterior sampling proposal

Alternatively, the previous decomposition defines a sequence of distributions

$$p_k^y(\mathrm{d}x_k) \propto g_k^y(x_k) p_k(\mathrm{d}x_k)\,, \quad k \in [\![0, n]\!]\,,$$

where the posterior of interest is the terminal distribution at $k = 0$.

- If we have a particle approximation of p_{k+1}^y then we can evolve it into a particle approximation of p_k^y $\rightsquigarrow$ we recursively build an empirical approximation of p_0^y.
- The choice of potentials $\{g_k^y\}_{k \in [\![0,n]\!]}$ is crucial; we need to ensure that p_k^y is close enough to p_{k+1}^y so that we can bridge the intermediate distributions efficiently.

Posterior sampling proposal: recursion

Consider the following particle approximation of p^y_{k+1}

$$p^{N,y}_{k+1} = \frac{1}{N} \sum_{i=1}^{N} \delta_{\xi^i_{k+1}} \,,$$

Recall that $p_k(\mathrm{d}x_k) = \int p_{k|k+1}(\mathrm{d}x_k|x_{k+1}) p_{k+1}(\mathrm{d}x_{k+1})$,

Posterior sampling proposal: recursion

Consider the following particle approximation of p^y_{k+1}

$$p^{N,y}_{k+1} = \frac{1}{N}\sum_{i=1}^{N} \delta_{\xi^i_{k+1}} \,,$$

Recall that $p_k(\mathrm{d}x_k) = \int p_{k|k+1}(\mathrm{d}x_k|x_{k+1})p_{k+1}(\mathrm{d}x_{k+1})$,

$$p^y_k(\mathrm{d}x_k) = \frac{\int \frac{g^y_k(x_k)}{g^y_{k+1}(x_{k+1})} p_{k|k+1}(\mathrm{d}x_k|x_{k+1})p^y_{k+1}(\mathrm{d}x_{k+1})}{\int \frac{g^y_k(z_k)}{g^y_{k+1}(z_{k+1})} p_{k|k+1}(\mathrm{d}z_k|z_{k+1})p^y_{k+1}(\mathrm{d}z_{k+1})} \;,$$

Posterior sampling proposal: recursion

Consider the following particle approximation of p^y_{k+1}

$$p^{N,y}_{k+1} = \frac{1}{N}\sum_{i=1}^{N} \delta_{\xi^i_{k+1}} \,,$$

Recall that $p_k(\mathrm{d}x_k) = \int p_{k|k+1}(\mathrm{d}x_k|x_{k+1})p_{k+1}(\mathrm{d}x_{k+1})$,

$$p^y_k(\mathrm{d}x_k) = \frac{\int \frac{g^y_k(x_k)}{g^y_{k+1}(x_{k+1})} p_{k|k+1}(\mathrm{d}x_k|x_{k+1})p^y_{k+1}(\mathrm{d}x_{k+1})}{\int \frac{g^y_k(z_k)}{g^y_{k+1}(z_{k+1})} p_{k|k+1}(\mathrm{d}z_k|z_{k+1})p^y_{k+1}(\mathrm{d}z_{k+1})} \,,$$

and hence

$$p^y_k(\mathrm{d}x_k) \propto \int \underbrace{\frac{\int g^y_k(z_k)p_k(\mathrm{d}z_k|x_{k+1})}{g^y_{k+1}(x_{k+1})}}_{:=\widetilde{\omega}_k(x_{k+1})} p^y_k(\mathrm{d}x_k|x_{k+1})p^y_{k+1}(\mathrm{d}x_{k+1}) \,,$$

where $p^y_k(\mathrm{d}x_k|x_{k+1}) \propto g^y_k(x_k)p_{k|k+1}(\mathrm{d}x_k|x_{k+1}) \rightarrow$ available in closed form if we use a Gaussian potential with mean linear in x_k.

Posterior sampling proposal: SMC approximation

$$p_k^y(\mathrm{d}x_k) = \int p_k^y(\mathrm{d}x_k|x_{k+1}) \frac{\widetilde{\omega}_k(x_{k+1}) p_{k+1}^y(\mathrm{d}x_{k+1})}{\int \widetilde{\omega}_k(z_{t+1}) p_{k+1}^y(\mathrm{d}z_{k+1})} ,$$

Assume $p_k^{N,y} = \frac{1}{N}\sum_{i=1}^N \delta_{\xi_{k+1}^i}$ is a particle approximation of $p_{k+1}^{N,y}$.

⇝ **Weight**:

$$p_k^{N,y}(\cdot) \approx \sum_{i=1}^N \frac{\widetilde{\omega}_k(\xi_{k+1}^i)}{\sum_{j=1}^N \widetilde{\omega}_k(\xi_{k+1}^j)} p_k^y(\cdot|\xi_{k+1}^i) .$$

⇝ **Resample**: Draw $A_{k+1}^{1:N} \overset{\text{iid}}{\sim} \text{Categorical}(\{\omega_k^j\}_{j=1}^N)$ where $\omega_k^j \propto \widetilde{\omega}_t(\xi_{k+1}^j)$.

⇝ **Mutate**: Sample $\xi_k^i \sim p_k^y(\cdot|\xi_{k+1}^{A_{k+1}^i})$ for $i \in [1:N]$,

$$p_k^{N,y} = \frac{1}{N}\sum_{i=1}^N \delta_{\xi_k^i} .$$

Gordon et al. (1993); Del Moral (2004); Cappe et al. (2005); Chopin et al. (2020)

Potentials: heuristic

For simplicity (and only in this slide) let $p_0(y)$ be the posterior of the inverse problem

$$Y = \overline{X}_0, \quad X_0 \sim p_0\,,$$

The marginals of the *forward process* initialized at p_0^y are

$$X_k \stackrel{\mathcal{L}}{=} \sqrt{\bar{\alpha}_k} X_0 + \sqrt{1 - \bar{\alpha}_k} Z, \quad X_0 \sim p_0^y, \quad Z \sim \mathcal{N}(\mathbf{0}_{d_x}, \mathrm{I}_{d_x})\,,$$

and so

$$\overline{X}_k \stackrel{\mathcal{L}}{=} \sqrt{\bar{\alpha}_k} y + \sqrt{1 - \bar{\alpha}_k}\, \overline{Z}\,, \quad \overline{Z} \sim \mathcal{N}(\mathbf{0}_{d_y}, \mathrm{I}_{d_y})\,.$$

- This suggests that one relevant choice of potentials is

$$g_k^y(x_k) = \mathcal{N}(\sqrt{\alpha_k} y; x_k, (1 - \alpha_k)\mathrm{I}_{d_y})\,.$$

Choice of potentials

- More generally, we let the variance be a free parameter $\sigma^2_{y,k}$.

Our proposal in the general case is

$$p^y_k(\mathrm{d}x_k) \propto g^y_k(x_k) p_k(\mathrm{d}x_k) \,, \quad g^y_k(x_k) := \mathcal{N}(\sqrt{\bar{\alpha}_k} y; A x_k, \sigma^2_{y,k} \mathrm{I}_{d_y})$$

- This particular choice of potential allows us to compute in closed form the auxiliary transition kernel $\propto g^y_k(x_k) p_{k|k+1}(\mathrm{d}x_k | x_{k+1})$ we use for our particle approximations.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

Illustration

⇝ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

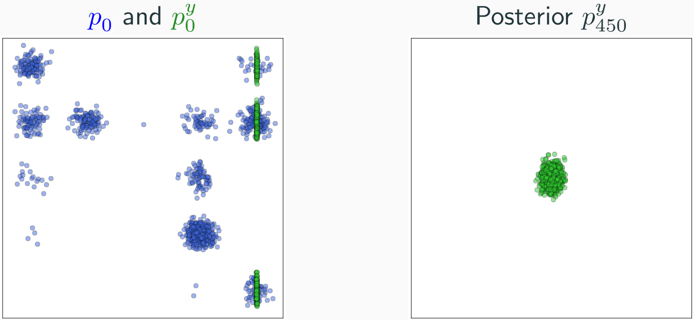


Figure 6: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

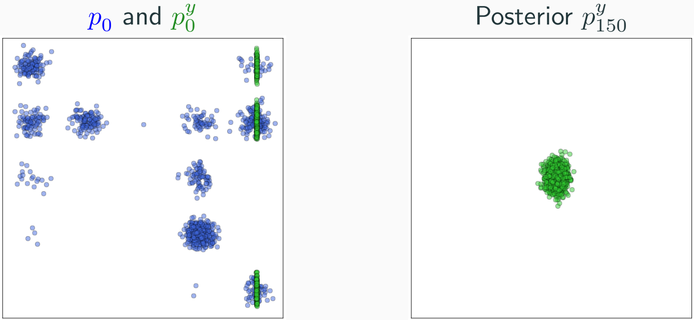


Figure 7: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

⇝ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

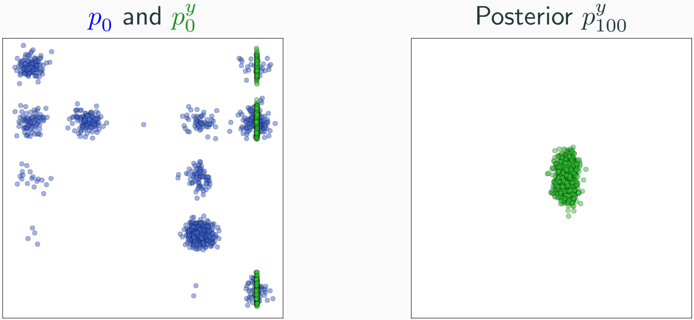


Figure 8: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

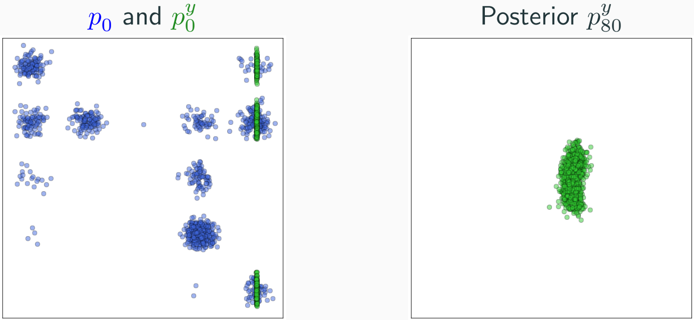


Figure 9: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

⇝ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

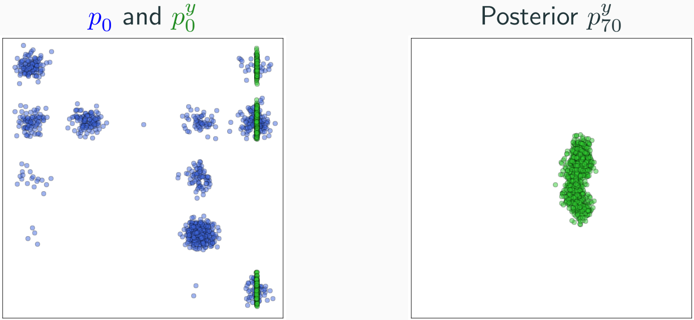


Figure 10: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

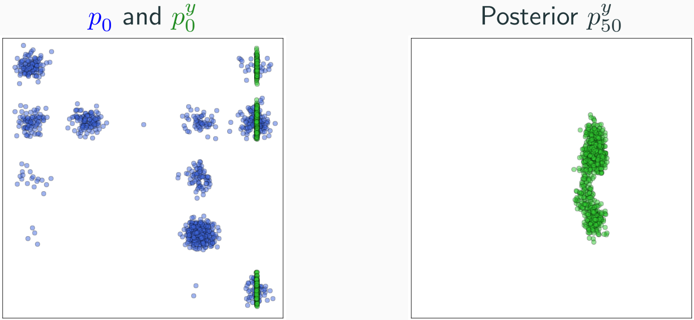


Figure 11: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

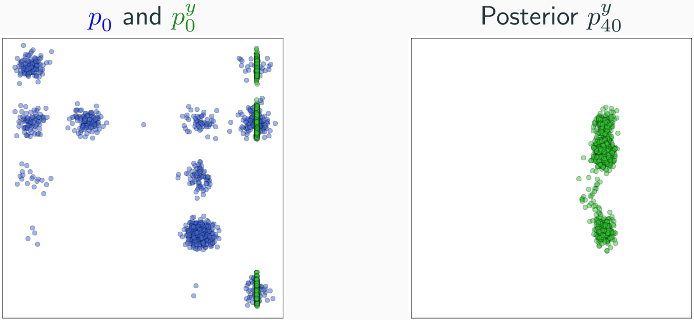


Figure 12: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow \{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

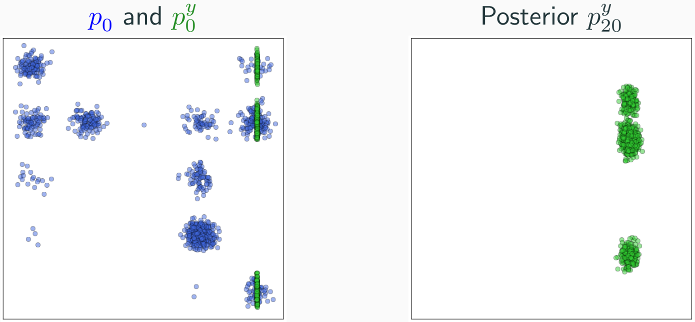


Figure 13: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

⇝ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

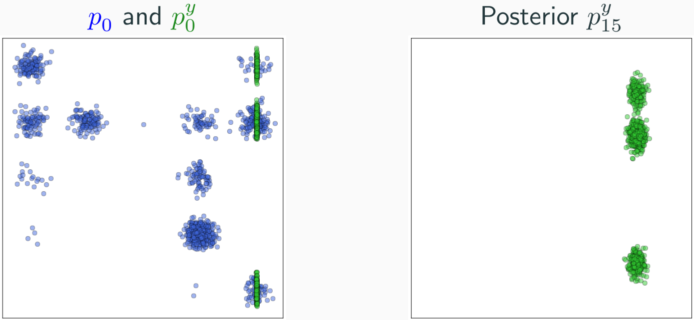


Figure 14: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

$\rightsquigarrow$ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

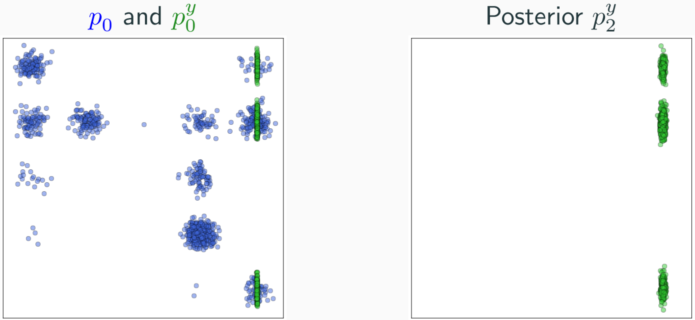


Figure 15: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

⇝ $\{p_k^y\}_{k=1}^n$ is available in closed form for the Gaussian mixture example.

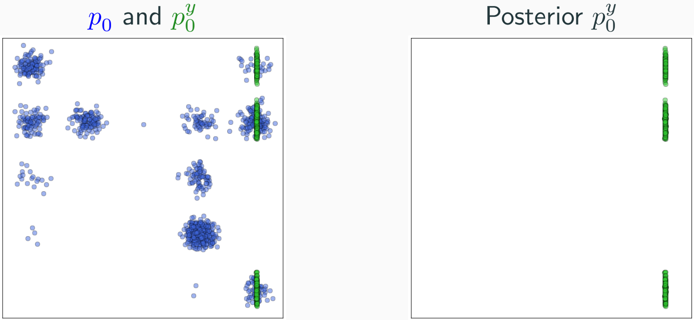


Figure 16: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Toy examples

$\rightsquigarrow$ 25 Gaussian mixture example with means

$$\mu_{i,j} = (8i, 8j, \ldots, 8i, 8j), \quad (i,j) \in \{-2, \ldots, 2\}$$

with unit convariance matrices. We randomly draw the weights of the mixture and the forward operator A and σ_y for the inverse problem $\rightsquigarrow$ $\nabla \log p_k$ is available in **closed form**.

$\rightsquigarrow$ 20 component mixture of translated and rotated Funnel distributions. We learn the score and consider the ground truth to be samples from parallel NUTS with very long chains.

Toy examples

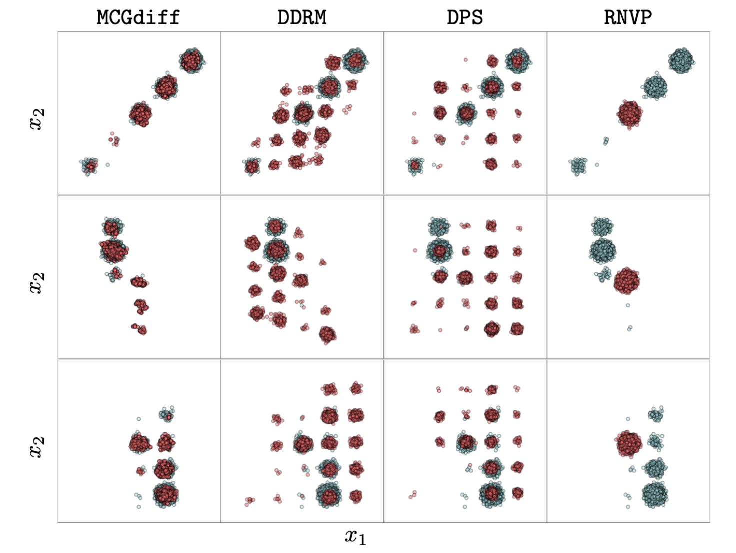
d	d_y	MCGdiff	DDRM	DPS	RNVP
80	1	**1.39 ± 0.45**	5.64 ± 1.10	4.98 ± 1.14	6.86 ± 0.88
80	2	**0.67 ± 0.24**	7.07 ± 1.35	5.10 ± 1.23	7.79 ± 1.50
80	4	**0.28 ± 0.14**	7.81 ± 1.48	4.28 ± 1.26	7.95 ± 1.61
800	1	**2.40 ± 1.00**	7.44 ± 1.15	6.49 ± 1.16	7.74 ± 1.34
800	2	**1.31 ± 0.60**	8.95 ± 1.12	6.88 ± 1.01	8.75 ± 1.02
800	4	**0.47 ± 0.19**	8.39 ± 1.48	5.51 ± 1.18	7.81 ± 1.63

d	d_y	MCGdiff	DDRM	DPS	RNVP
6	1	**1.95 ± 0.43**	4.20 ± 0.78	5.43 ± 1.05	6.16 ± 0.65
6	3	**0.73 ± 0.33**	2.20 ± 0.67	3.47 ± 0.78	4.70 ± 0.90
6	5	**0.41 ± 0.12**	0.91 ± 0.43	2.07 ± 0.63	3.52 ± 0.93
10	1	**2.45 ± 0.42**	3.82 ± 0.64	4.30 ± 0.91	6.04 ± 0.38
10	3	**1.07 ± 0.26**	4.94 ± 0.87	5.38 ± 0.84	5.91 ± 0.64
10	5	**0.71 ± 0.12**	2.32 ± 0.74	3.74 ± 0.77	5.11 ± 0.69

Figure 17: Sliced Wasserstein between samples of the target posterior and the empirical measure returned by each method. **Top**: Gaussian mixture. **Bottom**: Funnel mixture. We show the 95% CLT interval over 20 seeds.

DPS: Chung et al. (2023), DDRM: Kawar et al. (2022)

Toy examples

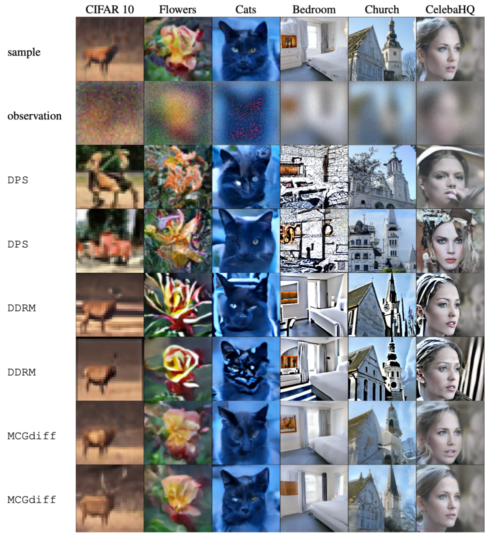


Imaging experiments

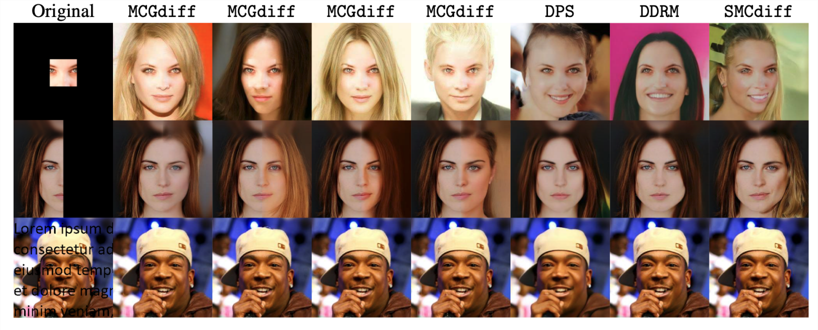
- $\rightsquigarrow$ Diffusion models learned on different datasets of image sizes varying from $(64, 64, 3)$ to $(256, 256, 3)$.
- $\rightsquigarrow$ We run parallel SMCs with $\mathbf{N = 64}$ particles.

Super-resolution example

Deblurring example



Inpainting example



Divide-and-conquer posterior sampling

Sequence of distributions

Let $(k_\ell)_{\ell=0}^L$ be an increasing sequence in $[\![0, n]\!]$ with $k_0 = 0$ and $k_L = n$.

Consider

$$p^y_{k_\ell}(\mathrm{d}x_{k_\ell}) \propto g^y_{k_\ell}(x_{k_\ell}) p_{k_\ell}(\mathrm{d}x_\ell)\,,$$

with

$$g^y_{k_\ell}(x_{k_\ell}) = \mathcal{N}(\sqrt{\alpha_{k_\ell}}\, y; Ax_{k_\ell}, \sigma^2_{y,k_\ell}\mathrm{I}_{d_y})\,.$$

- L is typically much smaller than n.
- This is the same sequence of distribution as in our SMC approach but now we only consider a small number L of intermediate distributions.
- Our goal is to recursively sample from each one of them without having to evolve N particles in parallel.
- We also want to solve the "image inconsistency" problem observed in our SMC method.

Recursion

Since

$$p_{k_\ell}(\mathrm{d}x_{k_\ell}) = \int \left\{ \prod_{j=k_\ell}^{k_{\ell+1}-1} p_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \right\} p_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}}) \,,$$

we can write $p^y_{k_\ell}$ in terms of forward smoothing kernels, i.e.

$$p^y_{k_\ell}(\mathrm{d}x_{k_\ell}) = \int \left\{ \prod_{j=k_\ell}^{k_{\ell+1}-1} p^{y,\ell}_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \right\} p^{y,\ell}_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}})$$

where

$$p^{y,\ell}_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}}) \propto \beta^{y,\ell}_{k_\ell|k_{\ell+1}}(x_{k_{\ell+1}})\, p_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}}) \,,$$
$$p^{y,\ell}_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \propto \beta^{y,\ell}_{k_\ell|j}(x_j)\, p_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \,,$$

and for all $j \in [\![k_\ell, k_{\ell+1}]\!]$

$$\beta^{y,\ell}_{k_\ell|j}(x_j) := \int g^y_{k_\ell}(x_{k_\ell}) p_{k_\ell|j}(\mathrm{d}x_{k_\ell}|x_j).$$

DCPS summary

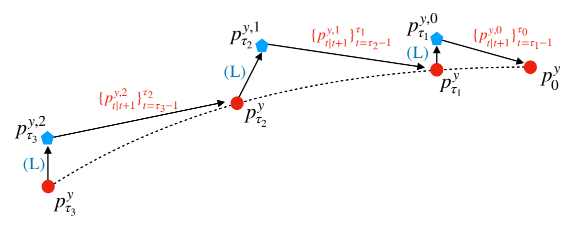


Figure 18: Illustration of idealized DCPS.

Starting at an approximate sample $X^y_{k_{\ell+1}}$ from $p^y_{k_{\ell+1}}$

- Use ULA initialized at $X^y_{k_{\ell+1}}$ to obtain an approximate sample from $X^{y,\ell}_{k_{\ell+1}}$.
- Starting from $X^{y,\ell}_{k_{\ell+1}}$, simulate a Markov chain with transition kernels $(p^{y,\ell}_{j|j+1})^{k_\ell}_{j=k_{\ell+1}-1}$
- Repeat until the posterior of interest is reached.

Backward function approximation

- The first source of intractability are the backward functions $\beta^{y,\ell}_{k_\ell|j}$.
- This is the same problem as before, however note that now they are expressed as an integral under $p_{k_\ell|j}(\cdot|x_j)$ with $j \in [\![k_\ell + 1, k_{\ell+1}]\!]$ instead of $p_{0|j}(\cdot|x_j)$ for $j \in [\![0, n]\!]$.
- This is more convenient since we expect Gaussian approximations of $p_{k_\ell|j}(\cdot|x_j)$ to be more accurate than those of $p_{0|j}(\cdot|x_j)$.

Backward kernel approximation

Assume again that forward=backward. Then for $j \in [\![k_\ell + 1, k_{\ell+1}]\!]$,

$$p_{k_\ell|j}(\mathrm{d}x_{k_\ell}|x_j) = \int q_{k_\ell|0,j}(\mathrm{d}x_{k_\ell}|x_0, x_j) p_{0|j}(\mathrm{d}x_0|x_j)\,,$$

Let $\hat{p}_{0|j}(\cdot|x_j)$ be an approximation of $p_{0|j}(\cdot|x_j)$ and define

$$\hat{p}_{k_\ell|j}(\mathrm{d}x_{k_\ell}|x_j) = \int q_{k_\ell|0,j}(\mathrm{d}x_{k_\ell}|x_0, x_j)\hat{p}_{0|j}(\mathrm{d}x_0|x_j)$$

- For `DPS` (Chung et al., 2023), $\hat{p}_{0|j}(\mathrm{d}x_0|x_j) = \delta_{\hat{x}^\theta_{0|j}(x_j)}(\mathrm{d}x_0)$.
- For Song et al. (2023), $\hat{p}_{0|j}(\mathrm{d}x_0|x_j) = \mathcal{N}(\mathrm{d}x_0; \hat{x}^\theta_{0|j}(x_j), r_j^2\,\mathrm{I}_{d_y})$.
- In both cases, $\hat{p}_{k_\ell|j}(\cdot|x_j)$ is computable in closed form. We write

  $$\hat{p}_{k_\ell|j}(\mathrm{d}x_{k_\ell}|x_j) = \mathcal{N}(\mathrm{d}x_{k_\ell}; \mu_{k_\ell|j}(x_j), \sigma^2_{k_\ell|j}\,\mathrm{I}_{d_x})\,.$$

  where both the mean and variance depend on the approximation used.

Backward kernel approximation

Proposition
Assume forward=backward. For all $\ell \in [\![0, L]\!]$, $j \in [\![k_\ell + 1, k_{\ell+1}]\!]$,

$$W_2(\hat{p}_{k_\ell|j}(\cdot|x_j), p_{k_\ell|j}(\cdot|x_j)) \leq \frac{\sqrt{\alpha_{k_\ell}}(1 - \alpha_j/\alpha_{k_\ell})}{1 - \alpha_j} W_2(\hat{p}_{0|j}(\cdot|x_j), p_{0|j}(\cdot|x_j)) \,.$$

where $\frac{\sqrt{\alpha_{k_\ell}}(1-\alpha_j/\alpha_{k_\ell})}{1-\alpha_j} < 1$ *and goes to* 0 *as* $j \to k_\ell$.

- We improve upon the previous approximations by performing Gaussian approximations on intervals $[\![k_\ell, k_{\ell+1}]\!]$ of moderate size.
- Our approximation of the backward function is then

$$\begin{aligned}\beta^{y,\ell}_{k_\ell|j}(x_j) \approx \hat{\beta}^{y,\ell}_{k_\ell|j}(x_j) &:= \int g^y_{k_\ell}(x_{k_\ell}) \hat{p}_{k_\ell|j}(\mathrm{d}x_{k_\ell}|x_j) \\ &= \mathcal{N}(\sqrt{\alpha_{k_\ell}}\, y; A\mu_{k_\ell|j}(x_j), \sigma^2_{k_\ell|j} AA^\intercal + \sigma^2_{y,\ell} \mathrm{I}_{d_y}) \,.\end{aligned}$$

FSK approximation

Recall that the quantities of interest are

$$p^{y,\ell}_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \propto \beta^{y,\ell}_{k_\ell|j}(x_j)\, p_{j|j+1}(\mathrm{d}x_j|x_{j+1})\,,$$
$$p^{y,\ell}_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}}) \propto \beta^{y,\ell}_{k_\ell|k_{\ell+1}}(x_{k_{\ell+1}})\, p_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}})\,.$$

Given the previous approximation of the backward function, we replace them instead with

$$\hat{p}^{y,\ell}_{j|j+1}(\mathrm{d}x_j|x_{j+1}) \propto \hat{\beta}^{y,\ell}_{k_\ell|j}(x_j)\, p_{j|j+1}(\mathrm{d}x_j|x_{j+1})\,,$$
$$\hat{p}^{y,\ell}_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}}) \propto \hat{\beta}^{y,\ell}_{k_\ell|k_{\ell+1}}(x_{k_{\ell+1}})\, p_{k_{\ell+1}}(\mathrm{d}x_{k_{\ell+1}})\,,$$

- Still, while now we can evaluate the density $\hat{p}^{y,\ell}_{j|j+1}(\cdot|x_{j+1})$ we still cannot sample from it.
- We can approximately sample from $\hat{p}^{y,\ell}_{k_{\ell+1}}$ using `ULA`.

Variational approximation I

For a fixed x_{j+1} we seek a mean-field Gaussian variational approximation of $\hat{p}^{y,\ell}_{j|j+1}(\cdot|x_{j+1})$ by solving

$$\underset{r^{y,\ell}_{j|j+1}(\cdot|x_{j+1}) \in \mathcal{G}_{\mathrm{D}}}{\operatorname{argmin}} \; \mathsf{KL}(r^{y,\ell}_{j|j+1}(\cdot|x_{j+1}) \parallel \hat{p}^{y,\ell}_{j|j+1}(\cdot|x_{j+1}))\,,$$

where $\mathcal{G}_{\mathrm{D}} := \{\mathcal{N}(\mu, \mathrm{diag}(\sigma)) : \mu \in \mathbb{R}^{d_x}, \sigma \in \mathbb{R}^{d_x}_{>0}\}$.

- We only learn vectors (μ, σ) that depend on the value of $X^{y,\ell}_{j+1}$ and do not seek to generalize as this incurs problem dependent, heavy training.

Variational approximation II

Letting $r^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1}) = \mathcal{N}(\mu^{y,\ell}_{j|j+1}, \mathrm{diag}(\mathrm{e}^{s^{y,\ell}_{j|j+1}}))$ where $s^{y,\ell}_{j|j+1} \in \mathbb{R}^{d_x}$,

$$
\begin{aligned}
&\mathsf{KL}(r^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1}) \parallel \hat{p}^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1})) \\
&= -\mathbb{E}\big[\log \hat{\beta}^{y,\ell}_{k_\ell|j}(\mu^{y,\ell}_{j|j+1} + \mathrm{diag}(\mathrm{e}^{s^{y,\ell}_{j|j+1}})Z)\big] + \frac{\|\mu^{y,\ell}_{j|j+1} - \mu_{j|j+1}(X^{y,\ell}_{j+1})\|^2}{2\sigma^2_{m|m+1}} \\
&\qquad - \frac{1}{2}\sum_{i=1}^{d_x}\left(s^{y,\ell}_{j|j+1,i} - \frac{\mathrm{e}^{s^{y,\ell}_{j|j+1,i}}}{\sigma^2_{m|m+1}}\right),
\end{aligned}
$$

- We perform the optimization using SGD.
- Crucially, we normalize the gradients to ensure the stability of the training procedure.
- In practice, we only perform 2 or 3 SGD steps.

Tamed ULA steps

We now turn to the Langevin steps on $\hat{p}^{y,\ell}_{k_{\ell+1}}$.

As the marginals $(p_k)_{k=0}^n$ approximate the true marginals of the forward process initialized at the data distribution π, we may use

$$s^\theta_k(x_k) = -(x_k - \sqrt{\alpha_k}\hat{x}^\theta_{0|k}(x_k))/(1-\alpha_k)\,,$$

as a substitute for $\nabla_{x_k} \log p_k(x_k)$, following Dhariwal and Nichol (2021).

We sample approximately from $\hat{p}^{y,\ell}_{k_{\ell+1}}$ by running M steps of the Tamed Unadjusted Langevin scheme (Brosse et al., 2019)

$$X_{j+1} = X_j + \gamma G^{y,\ell}_\gamma(X_j) + \sqrt{2\gamma} Z_j\,, \quad X_0 = X^y_{k_{\ell+1}}\,, \tag{1}$$

where

$$G^{y,\ell}_\gamma(x) := \frac{\nabla \log \hat{\beta}^{y,\ell}_{k_\ell|k_{\ell+1}}(x) + s^\theta_{k_{\ell+1}}(x)}{1 + \gamma \|\nabla \log \hat{\beta}^{y,\ell}_{k_\ell|k_{\ell+1}}(x) + s^\theta_{k_{\ell+1}}(x)\|}\,,$$

and set $X^{y,\ell}_{k_{\ell+1}} := X_M$.

Summary

Given an approximate sample $X^y_{k_{\ell+1}}$ from $\hat{p}^y_{k_{\ell+1}}$,

- Run `TULA` starting from $X^y_{k_{\ell+1}}$ to obtain $X^{y,\ell}_{k_{\ell+1}}$ approximately distributed according $\hat{p}^{y,\ell}_{k_{\ell+1}}$.
- Sample $(X^{y,\ell}_j)^{k_\ell}_{j=k_{\ell+1}}$: given $X^{y,\ell}_{j+1}$ with $j \in [\![k_\ell, k_{\ell+1} - 1]\!]$,
  - Find variational approximation $r^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1})$.
  - Draw $X^{y,\ell}_j \sim r^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1})$.
- Repeat these steps.

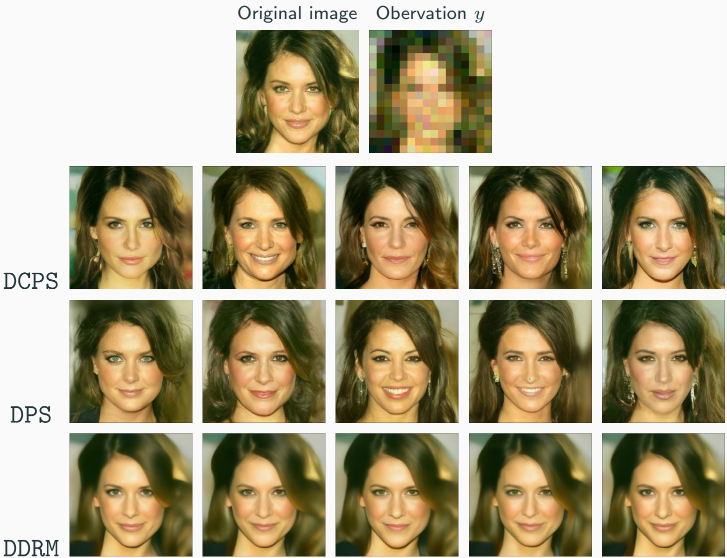
Toy experiments

- Same 25 Gaussian mixture example.
- $\texttt{DCPS}_M$ refers to our algorithm with M Langevin steps at the beginning of each block.
- We use $L = 4$.
- We also estimate the empirical weights of each Gaussian mixture mode and compare with the ground truth.

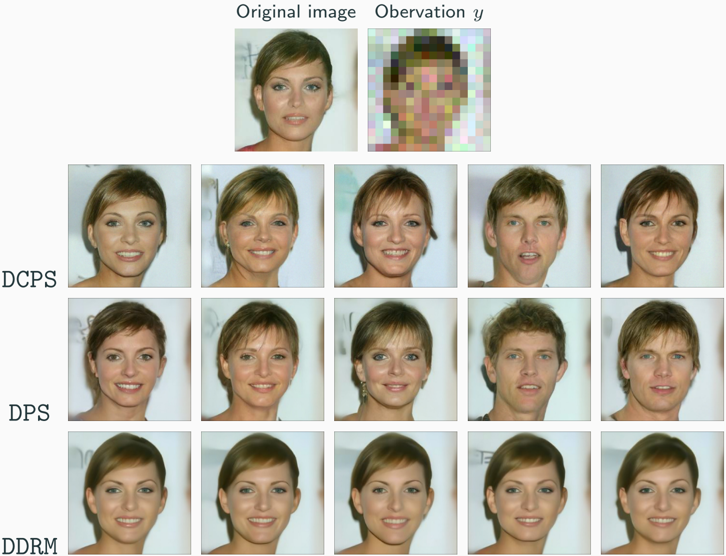
	$d_x = 10,\, d_y = 1$		$d_x = 100,\, d_y = 1$	
	SW	Δw	SW	Δw
MCGDiff	$2.25/2.69 \pm 2.07$	0.32 ± 0.20	$2.72/3.13 \pm 1.76$	0.42 ± 0.19
DPS	$3.12/5.64 \pm 8.45$	0.20 ± 0.12	$4.29/4.93 \pm 4.85$	0.35 ± 0.25
DDRM	$2.66/3.06 \pm 1.90$	0.36 ± 0.16	$5.97/6.26 \pm 2.33$	0.52 ± 0.19
$\texttt{DCPS}_{50}$	$1.95/2.70 \pm 2.28$	0.17 ± 0.25	$4.40/4.72 \pm 2.18$	0.44 ± 0.16
$\texttt{DCPS}_{500}$	$1.26/2.59 \pm 2.83$	0.13 ± 0.30	$2.81/3.22 \pm 2.21$	0.32 ± 0.18

Table 1: Results for the Gaussian mixture experiment. Results for the SW

Super-resolution experiments



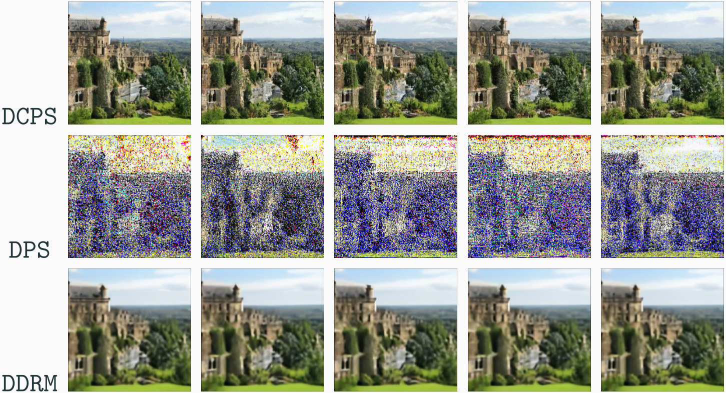
Super-resolution experiments



Super-resolution experiments

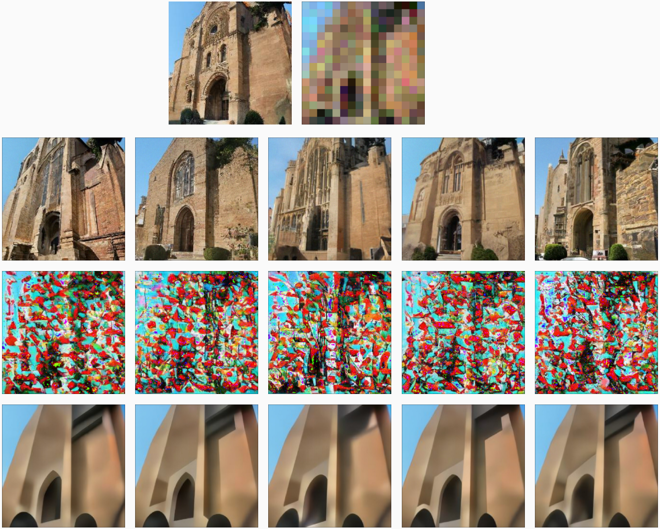
Original image

Obervation y



Super-resolution experiments

Original image Obervation y

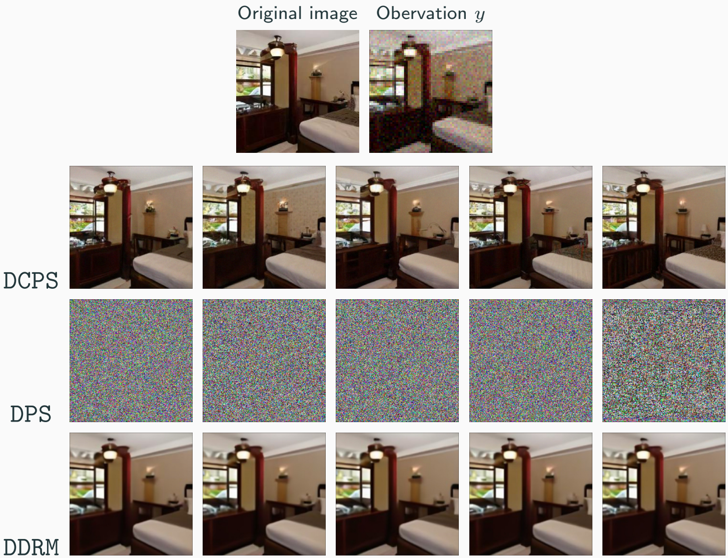


DCPS

DPS

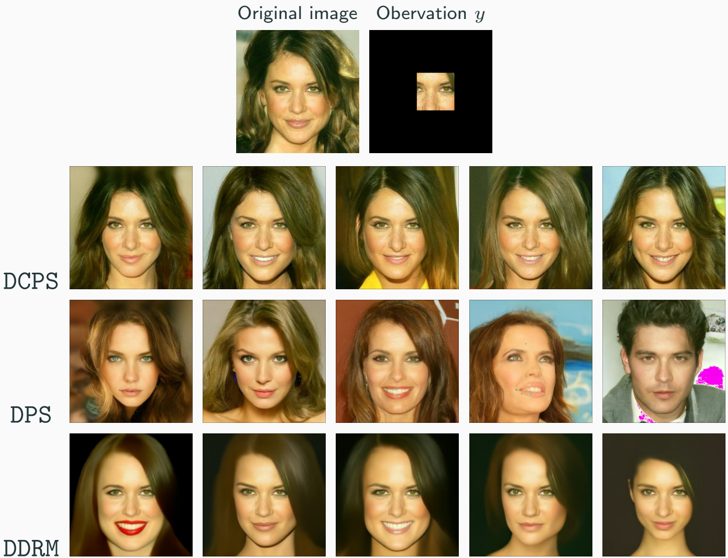
DDRM

Super-resolution experiments



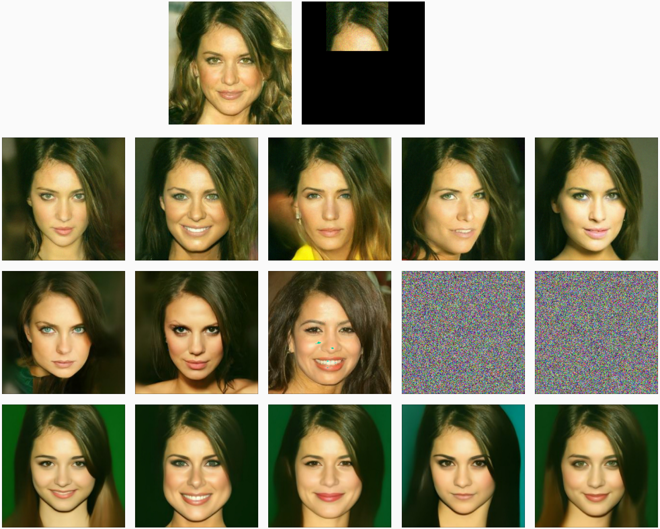
Super-resolution experiments

Inpainting and outpainting experiments



Inpainting and outpainting experiments

Original image Obervation y

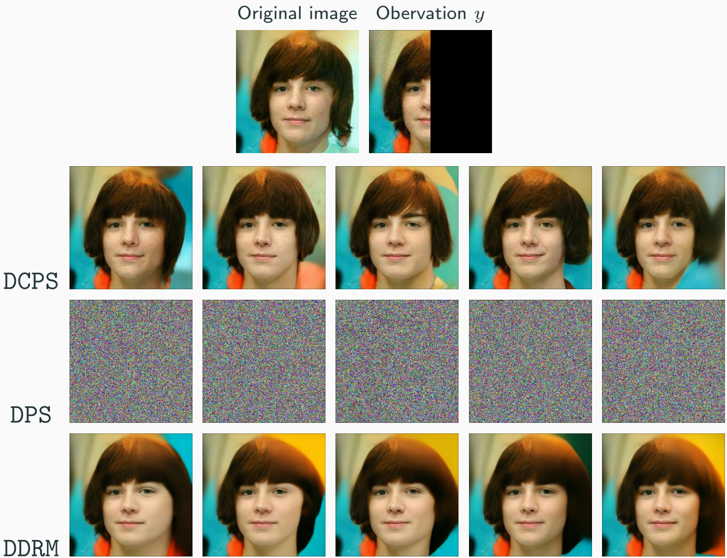


DCPS

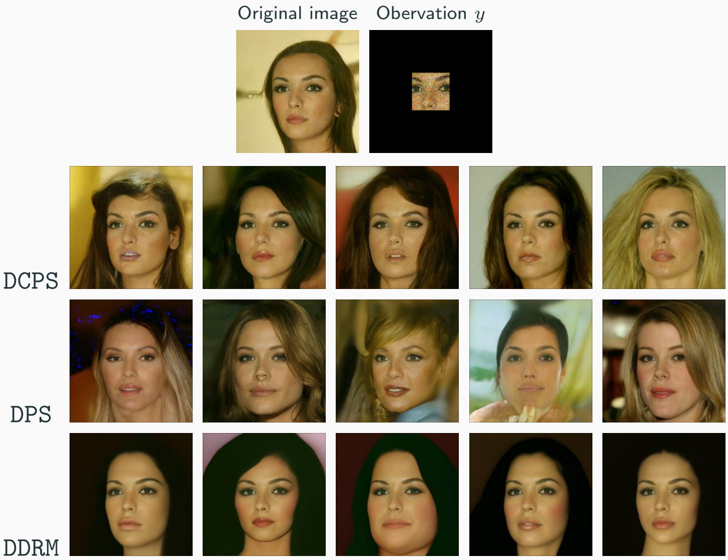
DPS

DDRM

Inpainting and outpainting experiments

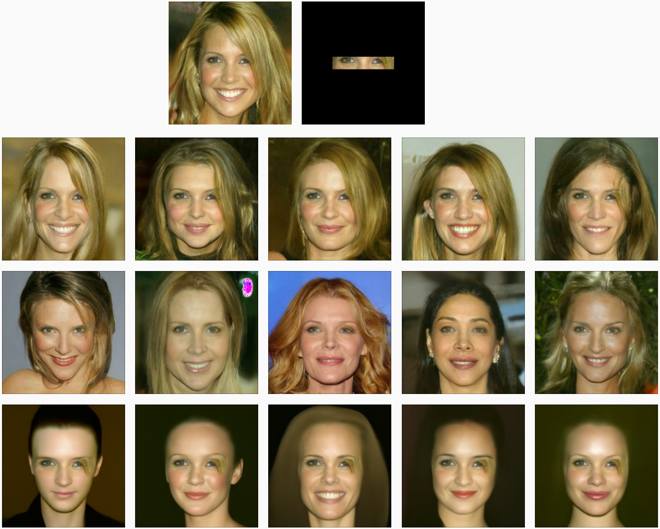


Inpainting and outpainting experiments



Inpainting and outpainting experiments

Original image Obervation y

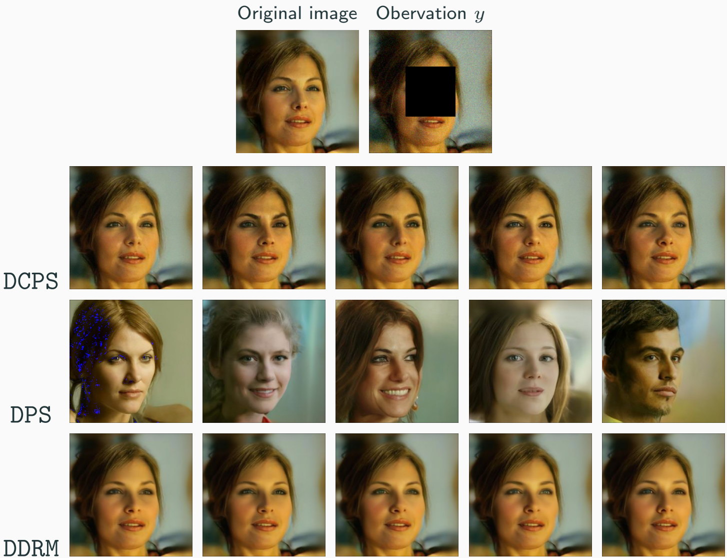


DCPS

DPS

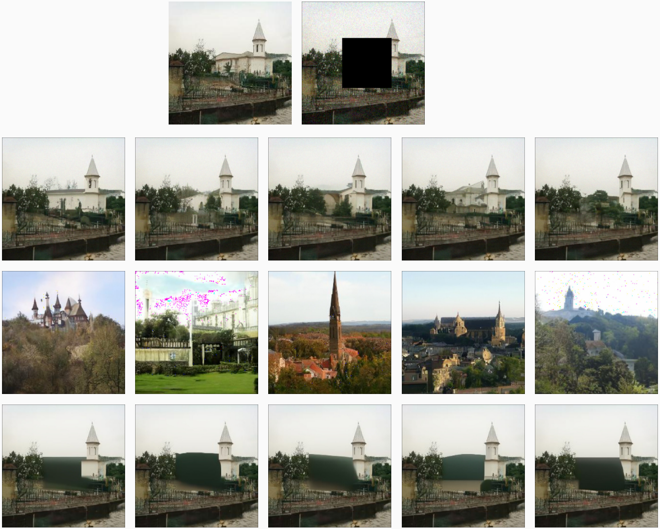
DDRM

Inpainting and outpainting experiments



Inpainting and outpainting experiments

Original image Obervation y



DCPS

DPS

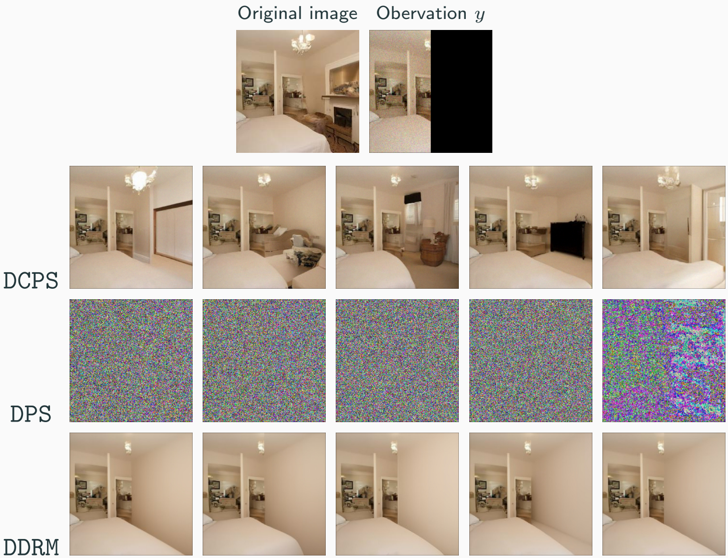
DDRM

Inpainting and outpainting experiments

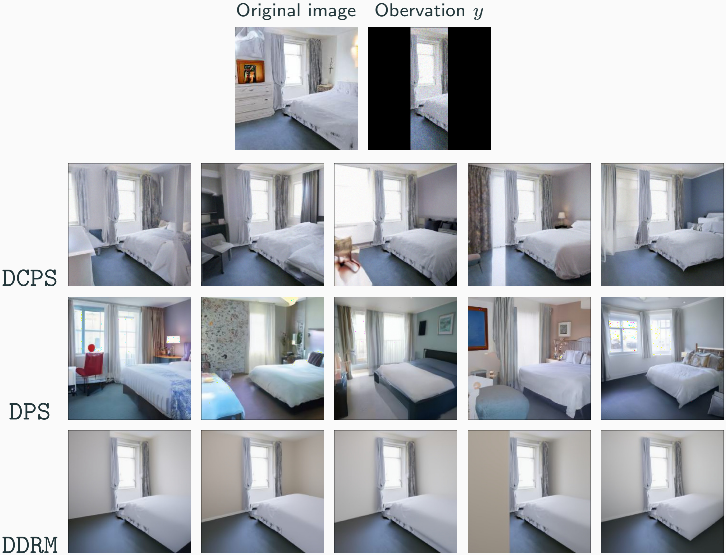
Inpainting and outpainting experiments

Inpainting and outpainting experiments

Inpainting and outpainting experiments



Inpainting and outpainting experiments



Colorization experiments

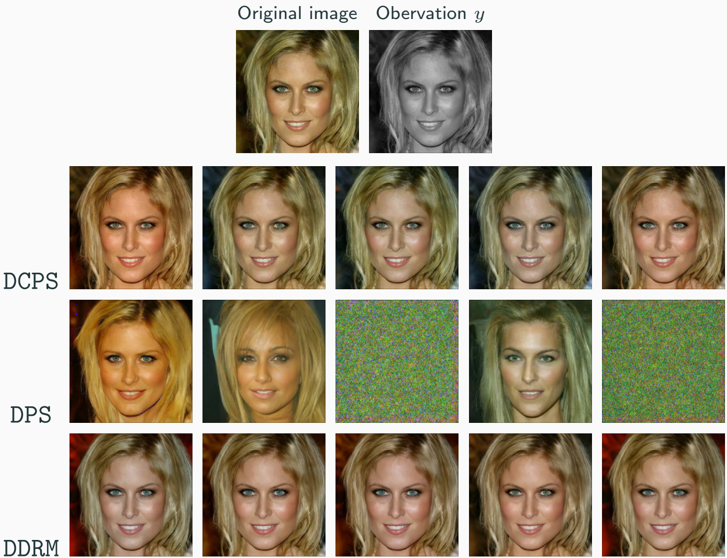
Original image Obervation y

DCPS

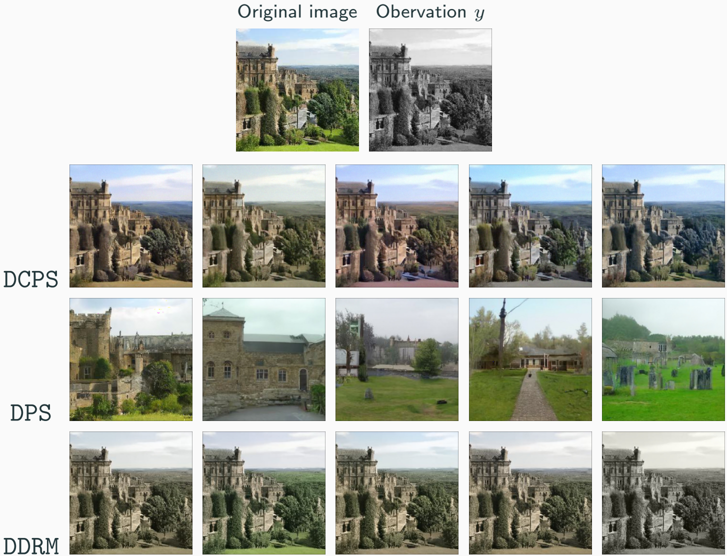
DPS

DDRM

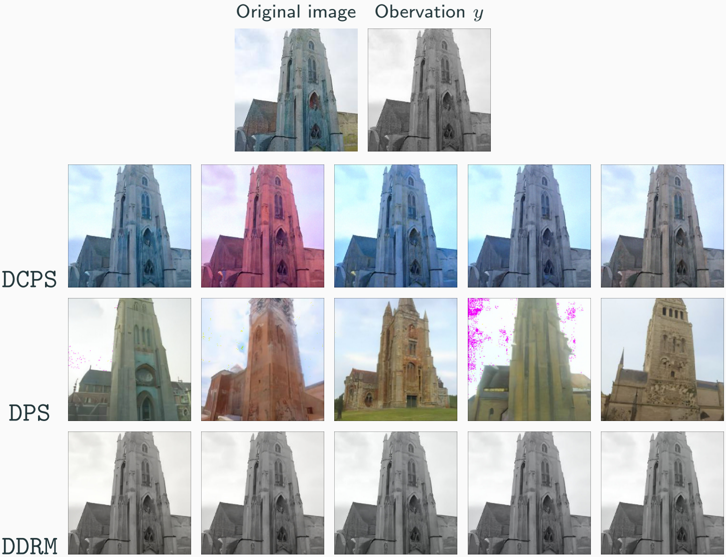
Colorization experiments



Colorization experiments



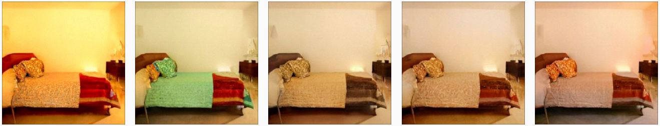
Colorization experiments



Colorization experiments

Original image   Obervation y

DCPS



DPS

DDRM

Thank you!

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