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 $X^i \in \mathbb{R}^{d_x}$.

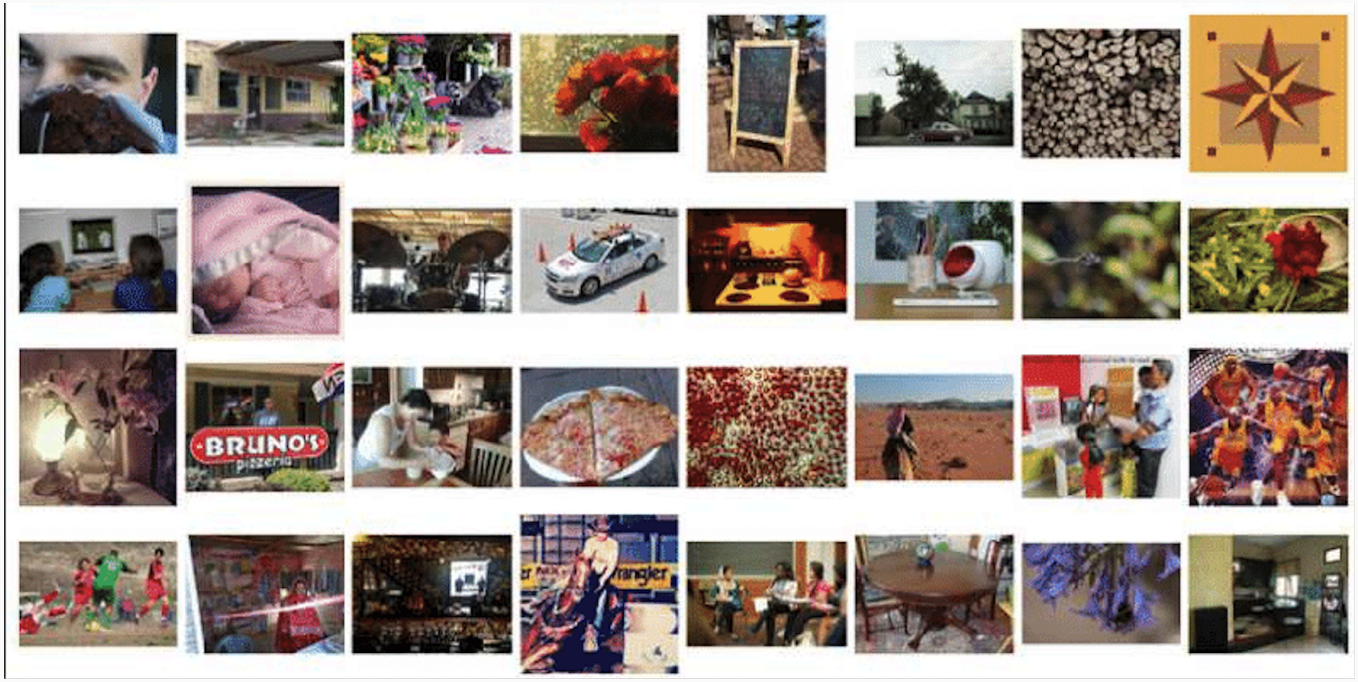

Figure 1: Samples from the `ImageNet` dataset.

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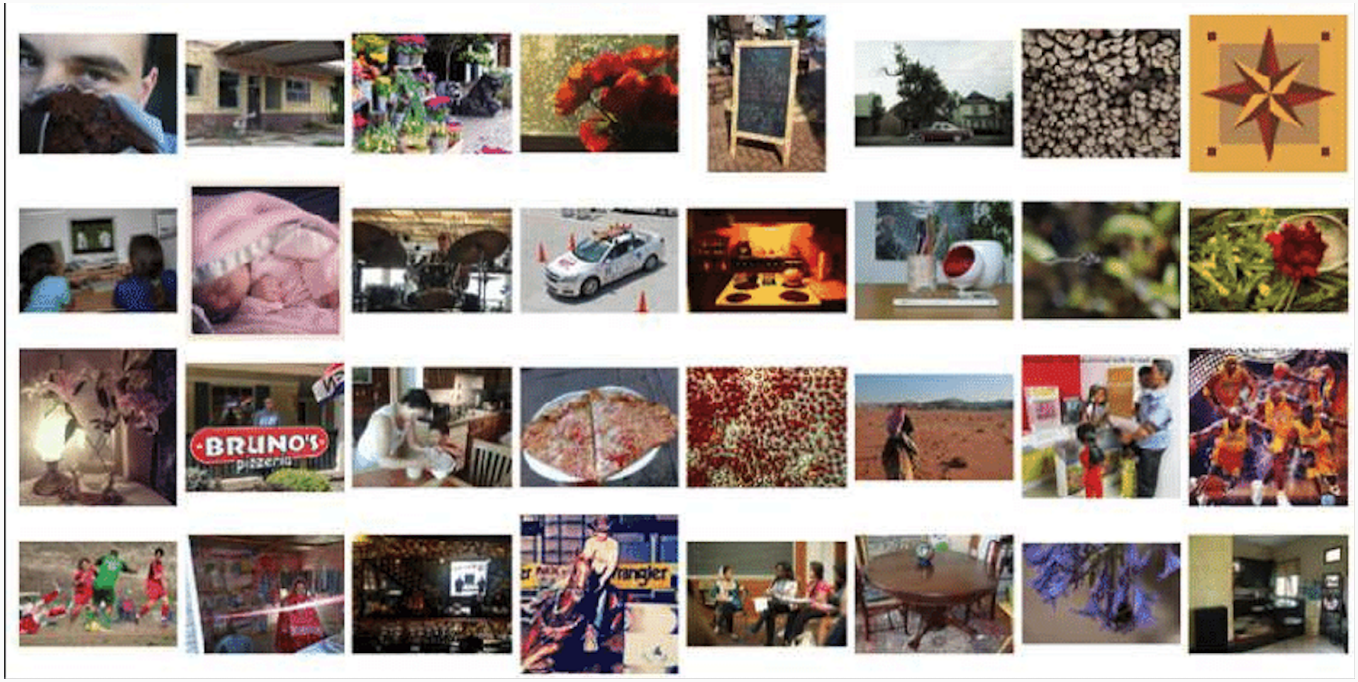

Figure 1: Samples from the `ImageNet` dataset.

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.

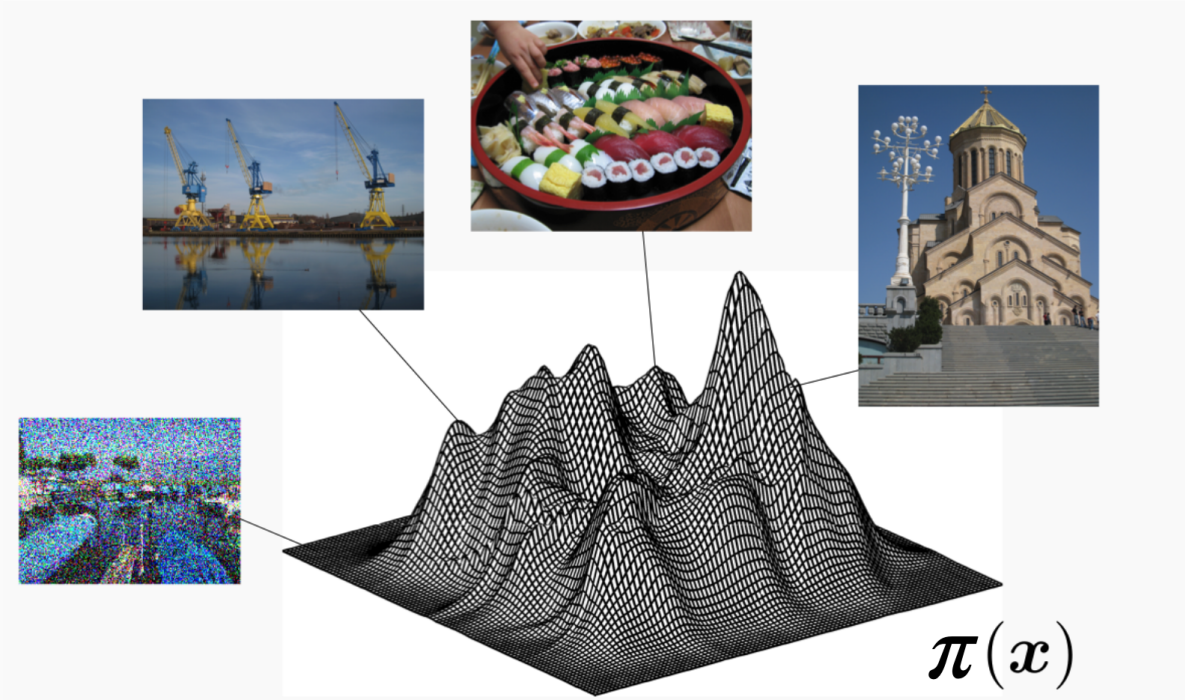

Figure 2: data distribution.

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 and Ermon (2020)

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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 $(X^1, \dots, X^N) \sim \pi$.

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

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

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

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

$\rightsquigarrow$ 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 $x_1, x_2 \dots x_T$ with transition kernel $q_{t|t-1}(\mathrm{d}x_t \mid x_{t-1})$.
- The joint distribution of $x_1, x_2 \dots x_T$ conditioned on x_0, denoted as $q_{0:T}(\mathrm{d}(x_1, \dots, x_T) \mid x_0)$, may be written as

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

- 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 $q_{t|0}\left(x_t \mid x_0\right)$ 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

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

- 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,

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

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 $\pi_{\mathrm{ref}}(x_T) = \mathcal{N}(x_T; \mathbf{0}, \mathrm{I})$ 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 $x_T \sim \pi_{\mathrm{ref}}(\cdot)$,
  - iteratively sample $x_{t-1} \sim p^{\theta}_{t-1|t}(\cdot \mid x_t)$ until $t = 1$.

Diffusion model principles

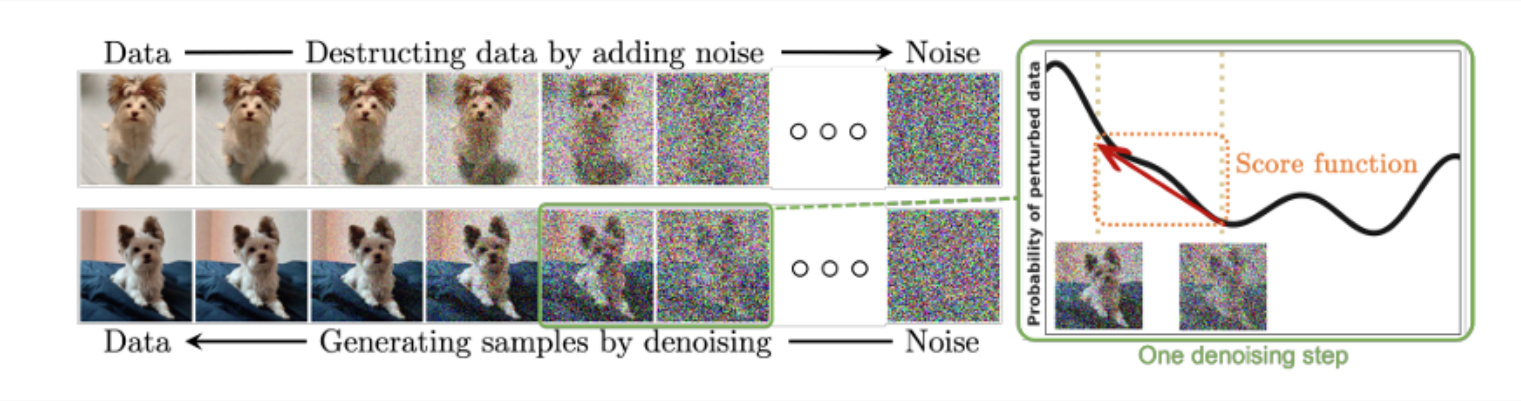

Figure 4: Diffusion models smoothly perturb data by adding noise, then reverse this process to generate new data from noise.

Variational Inference

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

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

  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:

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

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

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 $\Sigma_t^\theta(x_t) = \tilde{\beta}_t \mathrm{I}$,

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

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

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

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

$$\nabla_x \log q_t(x) = -\frac{x - \alpha_t \widehat{x}_{0|t}(x)}{\sigma_t^2}$$

where $\widehat{x}_{0|t}(x) = \mathbb{E}\left[X_0 | X_t = x\right]$ 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

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

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

$$s^{\theta}_t(x) = -\frac{x - \alpha_t \widehat{x}^{\theta}_{0|t}(x)}{\sigma_t^2}$$

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 $\mathrm{a} := \sigma\sigma^{\mathrm{t}}$, ($\sigma^{\mathrm{t}}$ is the transposed of σ.)

Assuming that the law of Y_t is absolutely continuous at each time t, under various hypotheses on b and a, one can prove that 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 anymore.

Time reversal formula for a diffusion process

Assumptions

- b is locally Lipschitz,
- a is bounded away from zero or that the derivative ∇a is well-behaved.

then

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

- 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.).

Summary

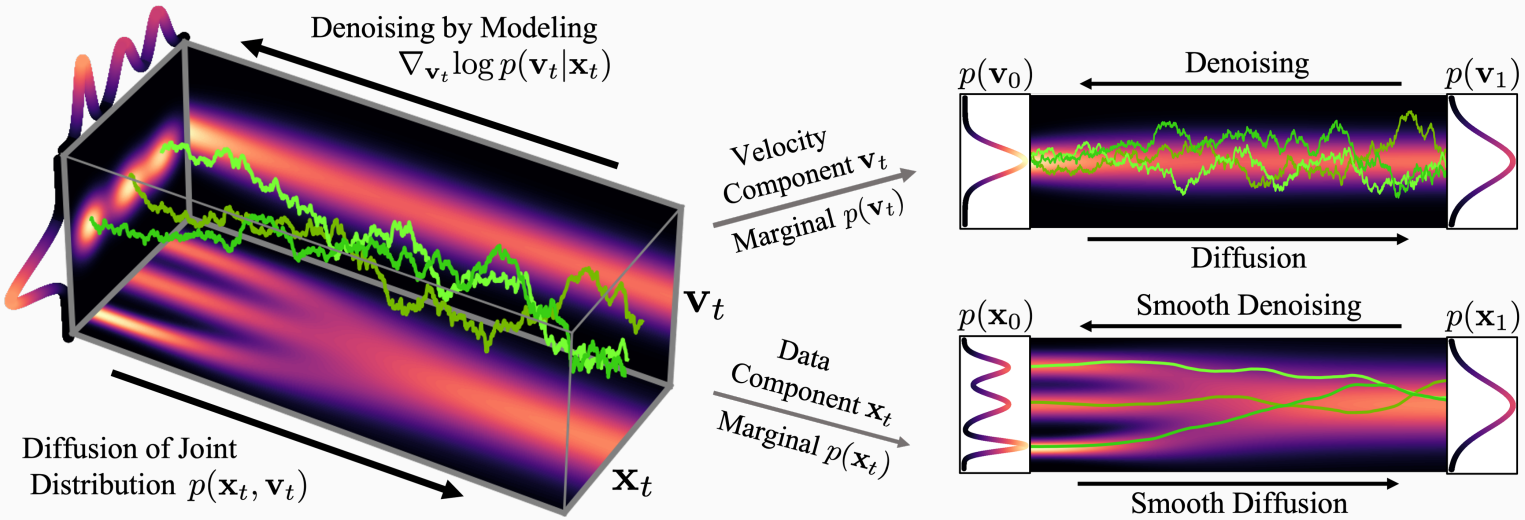

Figure 5: From Dockhorn et al. (2022)

Posterior Sampling

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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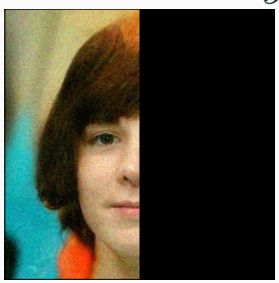
Sample from p_0

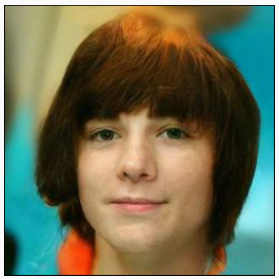
$\xrightarrow{AX+\sigma_y Z}$

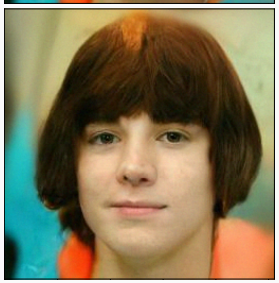
Observation y



$\longrightarrow$

Posterior samples





Inverse problems

Goal: Reconstruct an unknown $\mathbb{R}^{d_x}$-valued signal X from a $\mathbb{R}^m$-valued measurement Y based on a corruption model given by

$$Y = \mathcal{A}(X) + \sigma Z, \quad Z \sim \mathcal{N}(0, \mathrm{I}_m),$$

where $\mathcal{A}$ is the forward operator, Z is unobserved noise, and $\sigma > 0$ denotes the noise level.

- denoising, where $\mathcal{A}(x) = x$ and $\sigma > 0$ and the noise does not need to be Gaussian but can be heavy-tailed or even multiplicative;
- inpainting, where $\mathcal{A}(x) = Ax$ where A is a masking matrix with $A_{ij} = 0$ for $i \neq j$ and A_{ii} is either 0 or 1,
- deblurring, where $\mathcal{A}(x) = Ax$ where A is a 2D convolution operator (point spread function);
- phase retrieval, where $\mathcal{A}(x) = |Ax|$, where A is an invertible matrix.

Ill-posedness

- A key feature of these problems is that they are ill-posed, which means that some information is lost, making exact recovery impossible.
- In the Bayesian inverse problem framework, the solution is treated as a distribution. This approach represents unknown parameters as a random variables and updates the beliefs using Bayes' theorem based on the observed data.
- The Bayesian framework enables the incorporation of prior knowledge and the quantification of uncertainty, which is essential for addressing ill-posed problems
    - There is generally not a single solution compatible with the observations, but rather a set of solutions whose plausibility is measured by the posterior distribution.

Bayesian inverse problems

- In the Bayesian approach to inverse problems, we provide the unknown signal X with a prior distribution q.
- The likelihood function is expressed as

$$p(y|x) \propto \exp(-\|y - \mathcal{A}(x)\|^2/2\sigma^2).$$

- The goal is to sample from the posterior distribution $p(x|y) \propto p(y|x)q(x)$.
- This survey focuses on a specific class of methods that employ denoising diffusion models (DDMs) as priors. The goal is to sample reconstructions from the posterior $p(x|y)$ using models pre-trained with data from a given distribution, without the need for retraining or fine-tuning Song and Ermon (2019); Ho et al. (2020); Song et al. (2021b,a).

Bayesian inverse problems

- The setup we consider makes it possible, given a pre-trained DDM, to solve an arbitrary Bayesian inverse problem using this DDM as a prior, which eliminates the need to train a task-specific conditional model from scratch.
  - This is a departure from typical conditional DDM frameworks Song et al. (2021b); Batzolis et al. (2021); Tashiro et al. (2021); Saharia et al. (2022), which require access to a paired data set (X, Y) to learn a parametric approximation of the posterior distribution of the signal X given the observation Y.

Bayesian inverse problems

In the sequel we consider the problem of sampling approximately from some target distribution

$$\pi(\mathrm{d}x) := g(x)\mathsf{p}(\mathrm{d}x)/\mathcal{Z}$$

on $\mathbb{R}^{d_x}$, where

- g is some non-negative function on $\mathbb{R}^{d_x}$ referred to as the potential, which is assumed to be evaluable pointwise,
- p is a prior distribution, and $\mathcal{Z} := \int g(x)\mathsf{p}(\mathrm{d}x)$ is the normalising constant. We assume that p is provided by a DDM.

DDM prior

- A DDM prior imposes constraints that limit the flexibility in designing a sampler for the target posterior. First, recall that the posterior distribution π, depends on the prior p, which is intractable, and we only have access to its parametric approximation p^θ.
- Since p_0^θ represents the marginal of the latent variable model, we cannot directly evaluate its density or reliably approximate its score $\nabla \log p_0^\theta$.
- This makes it impractical to bridge between a standard Gaussian distribution and π via an annealing path for example; i.e., by considering an interpolation of the form $\pi_k \propto \pi^{\gamma_k} \mathcal{N}(\cdot; \mathbf{0}_{d_x}, \mathrm{I}_{d_x})^{1-\gamma_k}$, where $(\gamma_k)_{k=n}^0$ is a temperature schedule satisfying $\gamma_n = 0$ and $\gamma_0 = 1$ Syed et al. (2021); Dai et al. (2022).

DDM prior

- A natural approach to constructing a sampler for the posterior distribution π is to leverage the pretrained backward kernels $(p^{\theta}_{k|k+1}(x_k|x_{k+1}))_{k=0}^{n}$.
- We define the intermediate posterior distribution $\pi_k^*(x_k)$ as follows:

$$\pi_k^*(x_k) := \int q_{k|0}(x_k|x_0)\,\pi(\mathrm{d}x_0) = \int \frac{g(x_0)\mathsf{p}(\mathrm{d}x_0)}{\mathsf{p}(g)} q_{k|0}(x_k|x_0).$$

  This is the analogue of forward marginals, with the crucial difference being the replacement of p by π.

- However, unlike the marginal distribution of the forward process, $\mathsf{q}_k(\mathrm{d}x_k)$, sampling from this posterior distribution is intractable, as direct sampling from π is not possible.

Posterior sequence

- Idea: relate $\pi_k^*(x_k)$ to $\mathsf{q}_k(\mathrm{d}x_k)$ through the following expression:

$$\pi_k^*(x_k) = \frac{g_k(x_k)\mathsf{q}_k(x_k)}{\mathsf{q}_k(g_k)}, \quad \text{where} \quad g_k(x_k) = \int g(x_0) q_{0|k}(\mathrm{d}x_0|x_k).$$

  where we have set

$$q_{0|k}(\mathrm{d}x_0|x_k) := \mathsf{p}(\mathrm{d}x_0) q_{k|0}(\mathrm{d}x_k|x_0) / \mathsf{q}_k(x_k).$$

- The structure of π_k^* closely mirrors that of the posterior distribution π. Both are expressed as the product of the forward process's k-th marginal, q_k, and a potential function, which can be interpreted as the likelihood of the observation given the forward process at time k.

Conditional score and guidance terms

- The conditional scores $(\nabla \log \pi_k^*)_{k=1}^n$ can be obtained similarly with q_k replaced by

$$\nabla_{x_k} \log \pi_k^*(x_k) = \nabla_{x_k} \log \mathsf{q}_k(x_k) + \nabla_{x_k} \log g_k(x_k)\,.$$

- From Tweedie's formula, the conditional score is also related to the conditional denoiser $\mathbb{E}^\pi[X_0|X_k = x_k] = \int x_0\, \pi_{0|k}^*(\mathrm{d}x_0|x_k)$ where $\pi_{0|k}^*(\mathrm{d}x_0|x_k) \propto \pi(\mathrm{d}x_0) q_{k|0}(x_k|x_0)$.
  - The term $\nabla_{x_k} \log g_k(x_k)$, often referred to in the literature as the guidance term, indicates how the original score should be adjusted to steer the samples towards the posterior distribution.

Gradient guidance

- Idea: Approximate the denoiser $(x, k) \mapsto \mathbb{E}^{\pi}[X_0|X_k = x]$ where the conditional expectation is taken with respect to $\pi^*_{0|k}(\mathrm{d}x_0|x_k) \propto \pi(\mathrm{d}x_0)q_{k|0}(x_k|x_0)$.
- Key relation:

$$\mathbb{E}^{\pi}[X_0|X_k = x_k] = \mathbb{E}^{\mathsf{p}}[X_0|X_k = x_k] + \frac{1-\alpha_k}{\sqrt{\alpha_k}}\nabla_{x_k} \log g_k(x_k)$$

- Using an (unconditional) pre-trained denoisers $(x^{\theta}_{0|k})_{k=1}^n$, we can approximate the denoiser $\mathbb{E}^{\pi}[X_0|X_k]$ and enable approximate sampling from π using a DDPM-like approximation.

Gradient guidance

- A sample from the DDPM approximation of the posterior transition $\pi^*_{k|k+1}(\cdot|X_{k+1})$ is given by:

$$X_k = \widetilde{X}_k + \frac{v_{k+1|k}}{\sqrt{1 - v_{k+1|k}}} \widehat{\nabla \log g}_{k+1}(X_{k+1}), \quad \widetilde{X}_k \sim p^{\theta}_{k|k+1}(\cdot|X_{k+1}).$$

- Most of the methods mimick this update take the form:

$$X_k = \tilde{X}_{k+1} + \omega_k(X_{k+1}) \widehat{\nabla \log g}_{k+1}(X_{k+1}),$$

where ω_k is a weight function that varies according to the specific method.

Diffusion Posterior Sampling

- Chung et al. (2023) suggested to set

$$\nabla_{x_k} \log g_k(x_k) \approx \nabla_{x_k} \log g(x_{0|k}^{\theta}(x_k)) \,,$$

  which amounts to replace $q_{0|k}((|x_k)\mathrm{d}x_0)$ by $\delta_{x_{0|k}^{\theta} x_k}(\mathrm{d}x_0)$ in the definition the posterior.

- It involves the computation of a vector-Jacobian product involving the denoiser network since

$$\nabla_{x_k} \log g(x_{0|k}^{\theta}(x_k)) = \nabla_{x_k} x_{0|k}^{\theta}(x_k)^{\intercal} \nabla_{x_0} \log g(x_0)_{|x_0 = x_{0|k}^{\theta}(x_k)} .$$

- With $g(x) = \mathcal{N}_{d_y}(y; \mathcal{A}(x), {\sigma_y}^2 \mathrm{I})$, the update is

$$\omega_k(x_{k+1}) = \gamma {\sigma_y}^2 / \|y - \mathcal{A}(x_{0|k+1}^{\theta}(x_{k+1}))\| \,, \quad \gamma \in [0, 1] \,,$$

Gaussian approximation

- Song et al. (2023) proposed a Gaussian approximation:

$$q_{0|k}(x_0|x_k) \approx \mathcal{N}_{d_x}(x_0; x^{\theta}_{0|k}(x_k), v_{0|k}\mathrm{I}),$$

  where the variance $v_{0|k}$ is treated as a hyperparameter.

- Song et al. (2023) recommend setting $v_{0|k} = 1 - \alpha_k$, which matches the variance of $q_{0|k}(x_0|x_k)$ under the assumption that p is a standard Gaussian distribution.

  - For the specific case of linear inverse problems, where $g(x) = \mathcal{N}_{d_y}(y; Ax, {\sigma_y}^2\mathrm{I})$, the following approximation is employed.

$$\nabla_{x_k} \log g_k(x_k) \approx \nabla_{x_k} \log \mathcal{N}_{d_y}(y; Ax^{\theta}_{0|k}(x_k), v_{0|k}AA^{\intercal} + {\sigma_y}^2\mathrm{I})$$

    which is obtained by integrating g against the Gaussian approximation (**??**) using (Bishop, 2006, Formula 2.115).

Improved Gaussian approximation

- The vanilla Gaussian approximation can be further improved: note that the covariance is not related to the data distribution.
- In Finzi et al. (2023); Boys et al. (2023), it is suggested to solve the following optimization problem:

$$\underset{\mu \in \mathbb{R}^{d_x},\, \Sigma \in \mathcal{S}_{++}^{d_x}}{\operatorname{argmin}} \quad \mathsf{KL}(\mathcal{N}_{d_x}(\cdot; \mu, \Sigma) \parallel q_{0|k}(\cdot|x_k))\,,$$

  where $\mathcal{S}_{++}^{d_x}$ is the set of positive definite matrices.
- Using (Bishop, 2006, Section 10.7), the optimal solution, known as *moment projection*, is given by

$$\mu_{0|k}(x_k) = \mathbb{E}[X_0|X_k = x_k]\,, \quad \Sigma_{0|k}(x_k) = \mathbb{C}\mathrm{ov}[X_0|X_k = x_k]\,.$$

Feynman-Kac representation

- Although the sequence $(\pi_k^*)_{k=n}^0$ of distributions is a natural choice, this approach poses numerical challenges, as it involves quantities that are difficult to approximate.
- Alternative sequences can be explored, and as long as there is a way to transition effectively from the $(k+1)$th distribution to the kth one, accurate samples from the final distribution π can still be obtained.
- This is a well-proven strategy that has been extensively explored; see, *e.g.*, Gelman and Meng (1998); Del Moral (2013); Dai et al. (2022) .

Feynman-Kac representation

Given a generic sequence $(\pi_k)_{k=n}^0$ of distributions, a common approach involves establishing a recursive relationship between successive distributions π_{k+1} and π_k, such as

$$\pi_k(\mathrm{d}x_k) = \frac{1}{\mathcal{Z}_k} \int m_{k|k+1}(\mathrm{d}x_k \mid x_{k+1}) w_k(x_k, x_{k+1}) \pi_{k+1}(\mathrm{d}x_{k+1}),$$

where

- w_k is a non-negative weight function,
- $\mathcal{Z}_k = \int m_{k|k+1}(\mathrm{d}x_k \mid x_{k+1}) w_k(x_k, x_{k+1}) \pi_{k+1}(\mathrm{d}x_{k+1})$ is a normalising constant,
- $m_{k|k+1}(\cdot|x_{k+1})$ is a Markov kernel.

Sequential Monte Carlo I

- There are various approaches for sampling from a sequence of distributions satisfying

$$\pi_k(\mathrm{d}x_k) = \frac{1}{\mathcal{Z}_k} \int m_{k|k+1}(\mathrm{d}x_k \mid x_{k+1}) w_k(x_k, x_{k+1}) \pi_{k+1}(\mathrm{d}x_{k+1}),$$

- The most straightforward approach is to sequential Monte Carlo (SMC) methods (a.k.a. particle filters) is to approximate each distribution π_k in the sequence of interest by a weighted sample $(\omega_k^i, \xi_k^i)_{i=1}^N$ of random draws (the ξ_k^i's), referred to as particles, and associated non-negative importance weights (the ω_k^i's).

Sequential Monte Carlo II

- An SMC algorithm recursively propagates the weighted particle sample from one time step k to the next using importance sampling and resampling techniques, providing an approximation of π_k at each step.
- The particle samples serve two key purposes:
  - first, they can be used to approximate integrals with respect to the target distributions, which allows for estimates of relevant statistics;
  - second, since each particle represents a possible state of the Feynman–Kac flow, the weighted particle samples represent the distributions themselves, enabling inference at subsequent time steps. We refer to Chopin et al. (2020); Del Moral (2004); Del Moral (2013).

SMC for Feynman-Kac I

- Assume that we have access to a sample $(\omega_{k+1}^i, \xi_{k+1}^i)_{i=1}^N$ of particles and associated weights, the weighted empirical distribution π_{k+1}^N of which approximates π_{k+1}.
- In order to form an updated sample $(\omega_k^i, \xi_k^i)_{i=1}^N$ approximating π_k, we simply plug π_{k+1}^N into the FK recursion

$$\pi_k(\mathrm{d}x_k) = \frac{1}{\mathcal{Z}_k} \int m_{k|k+1}(\mathrm{d}x_k \mid x_{k+1}) w_k(x_k, x_{k+1}) \pi_{k+1}(\mathrm{d}x_{k+1}),$$

- This yields a mixture approximating π_k.

$$\bar{\pi}_k^N(\mathrm{d}x_k) \propto \sum_{i=1}^N \omega_{k+1}^i w_k(x_k, \xi_{k+1}^i)\, m_k(\mathrm{d}x_k \mid \xi_{k+1}^i)$$

SMC for Feynman-Kac II

- New particles are sampled from $\bar{\pi}_k^N$ using importance sampling based on some mixture proposal

$$\rho_k^N(\mathrm{d}x_k) \propto \sum_{i=1}^{N} \varphi_{k+1}^i \omega_{k+1}^i \, r_k(\mathrm{d}x_k \mid \xi_{k+1}^i),$$

  - r_k is some transition density dominating m_k
  - $(\varphi_{k+1}^i)_{i=1}^N$ is a set of positive weights referred to as adjustment multipliers Pitt and Shephard (1999).

SMC for Feynman-Kac III

(i) Draw indices $(\kappa_k^\ell)_{\ell=1}^N$ (conditionally) independently from the categorical distribution on $\{1, \ldots, N\}$ formed by the adjusted particle weights $(\omega_{k+1}^\ell \varphi_{k+1}^\ell)_{\ell=1}^N$;

(ii) Generate independently, for all sampled mixture indices, new particles $\xi_k^i \sim r_k(\mathrm{d}x_k \mid \xi_{k+1}^{\kappa_k^i})$;

(iii) Assign each new particle ξ_k^i an updated weight

$$\omega_k^i := w_k(\xi_k^i, \xi_{k+1}^{\kappa_k^i})(\mathrm{d}m_k/\mathrm{d}r_k)(\xi_k^i, \xi_{k+1}^{\kappa_k^i})/\varphi_k^{\kappa_k^i},$$

where $\mathrm{d}m_k/\mathrm{d}r_k$ denotes the Radon–Nikodym derivative of m_k w.r.t. r_k (which is well defined).

SMC for Feynman-Kac IV

- The sampling of the mixture indices (Step (i)) in can be equivalently understood as resampling, with replacement, new particles among the old ones in proportion to the adjusted weights.
- The sampling step (ii) serves to randomly jitter, or shake, the particles. We will therefore refer to operations (i–iii) collectively as the (resample–shake–weight) scheme (in the literature, operations (i) and (ii) are also often referred to as selection and mutation, respectively).

SMC for Feynman-Kac V

In some situations, the weight function w_k does not depend on x_k; in that case, we may sample exactly from $\bar{\pi}_k^N$, without the need of importance sampling, by instead

(i') computing the weights $(w_k(\xi_{k+1}^i)\omega_{k+1}^i)_{i=1}^N$;

(ii) drawing independently mixture indices $(\kappa_k^\ell)_{\ell=1}^N$ from the categorical distribution on $\{1, \ldots, N\}$ induced by the weights in (i');

(ii) generating new particles $\xi_k^i \sim m_k(\mathrm{d}x_k \mid \xi_{k+1}^{\kappa_{k+1}^i})$.

Appealingly, this procedure, which we refer to as the (weight–resample–shake) scheme, will always generate uniformly weighted particles at all iterations.

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).

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

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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

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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 $p_{k+1}^{N,y}$.

$\rightsquigarrow$ **Weight:**

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

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

$\rightsquigarrow$ **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

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

and so

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

- 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

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

- 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.

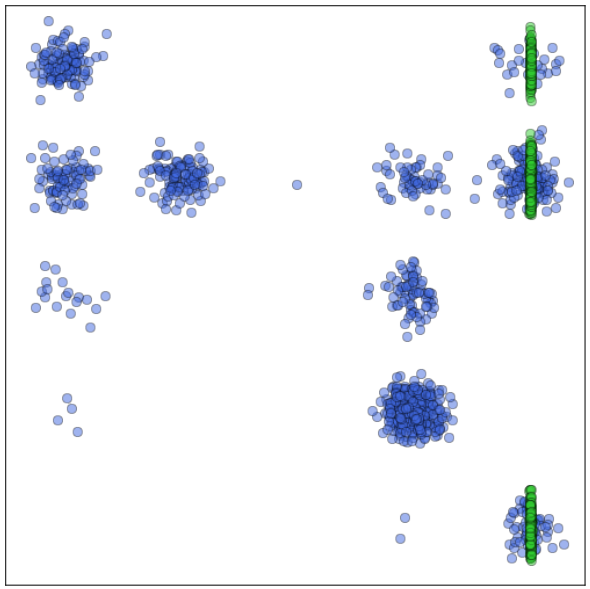
Illustration

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

Illustration

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

p_0 and p_0^y



Posterior p_{450}^y

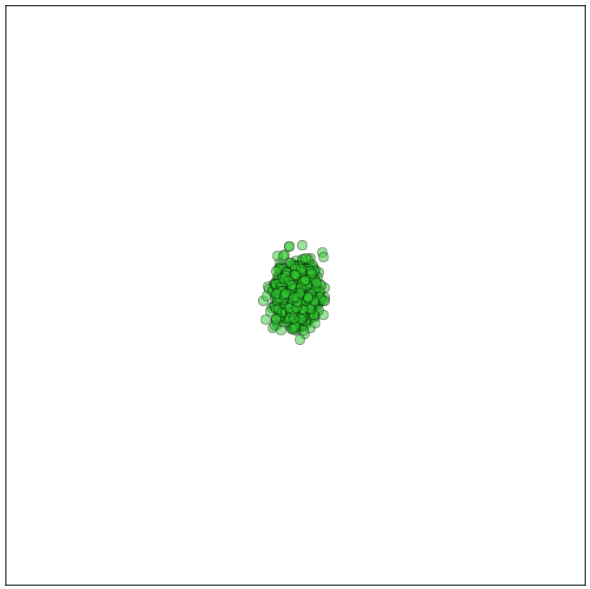


Figure 6: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

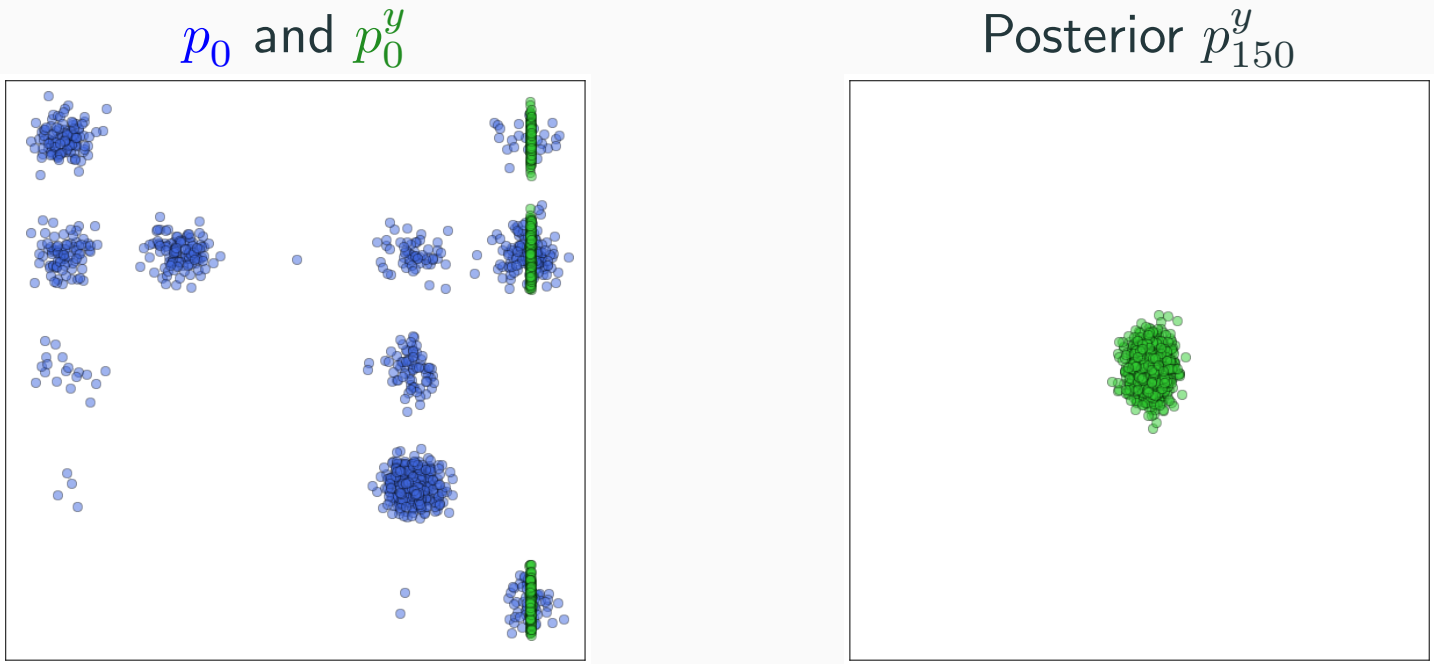
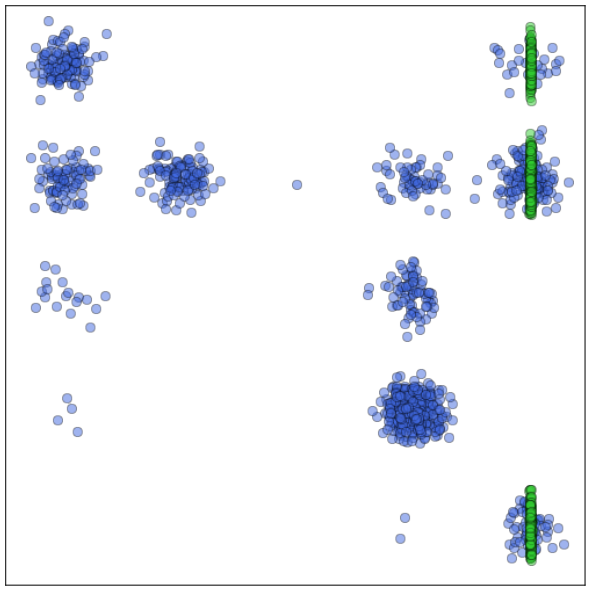


Figure 7: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

p_0 and p_0^y



Posterior p_{100}^y

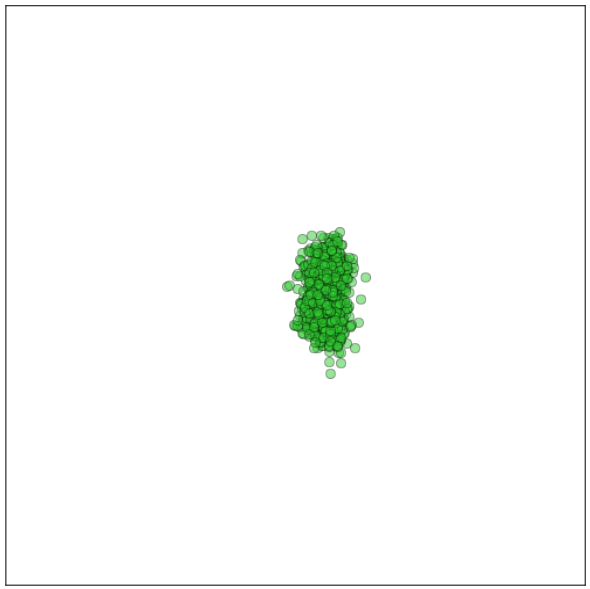
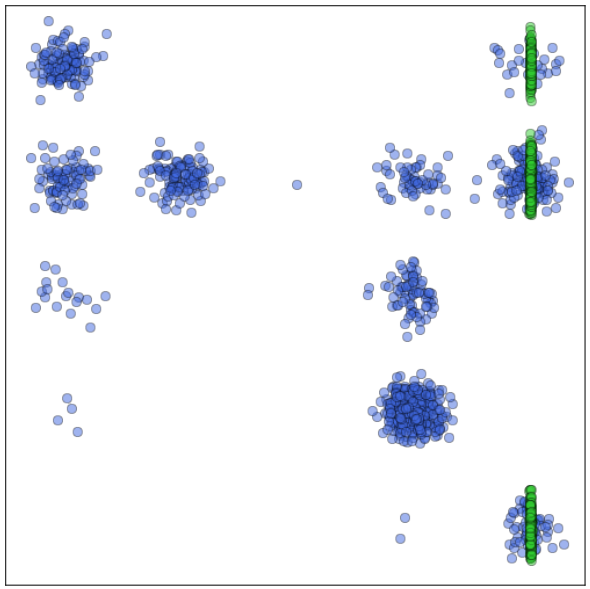


Figure 8: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

p_0 and p_0^y



Posterior p_{80}^y

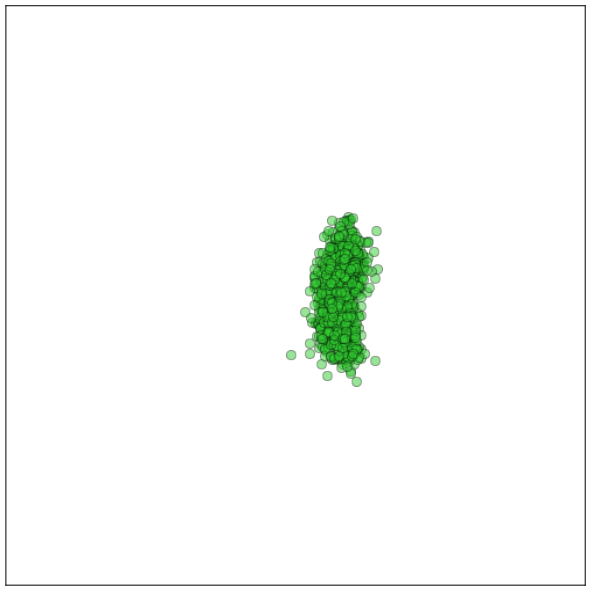


Figure 9: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

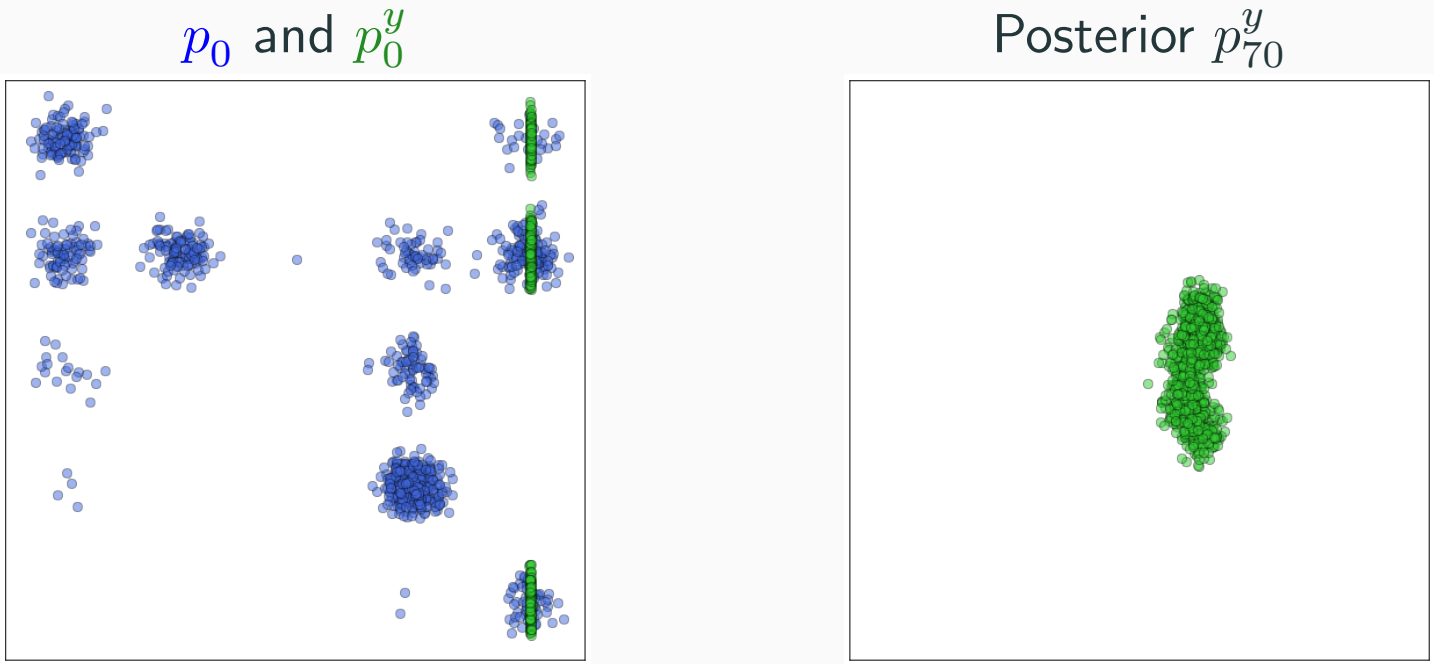


Figure 10: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

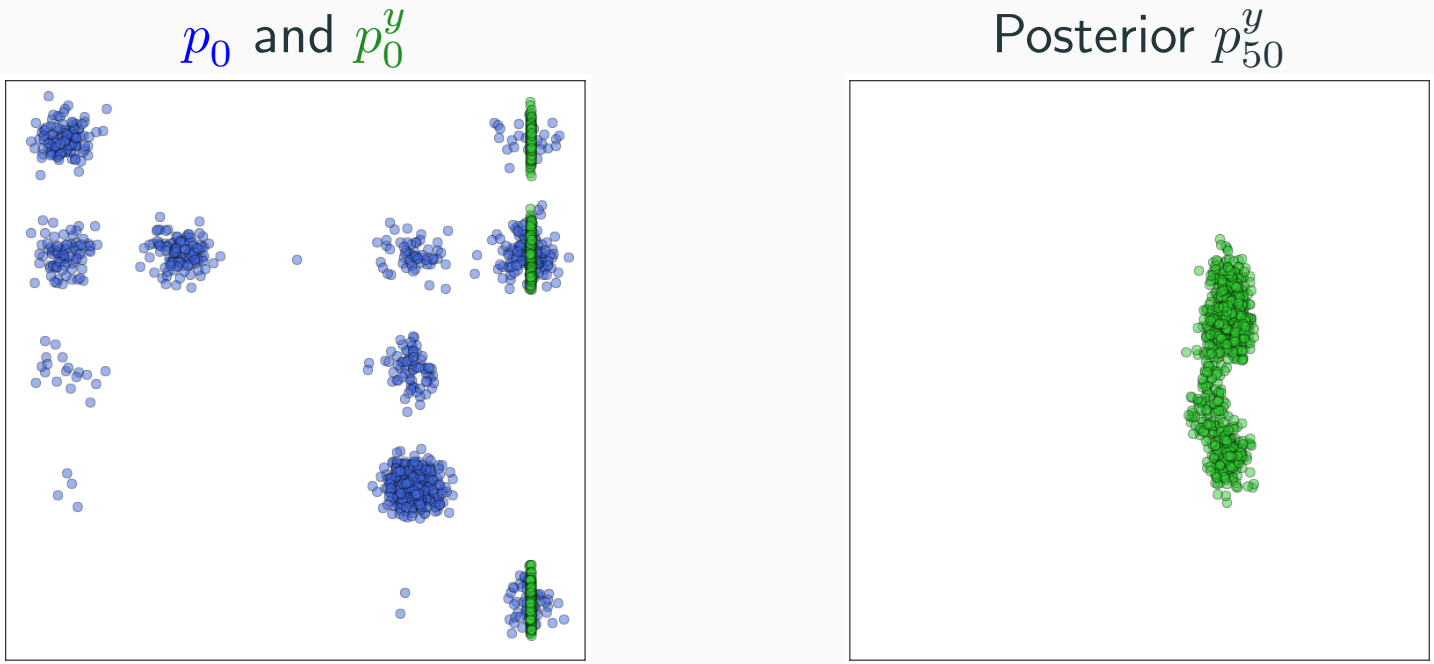


Figure 11: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

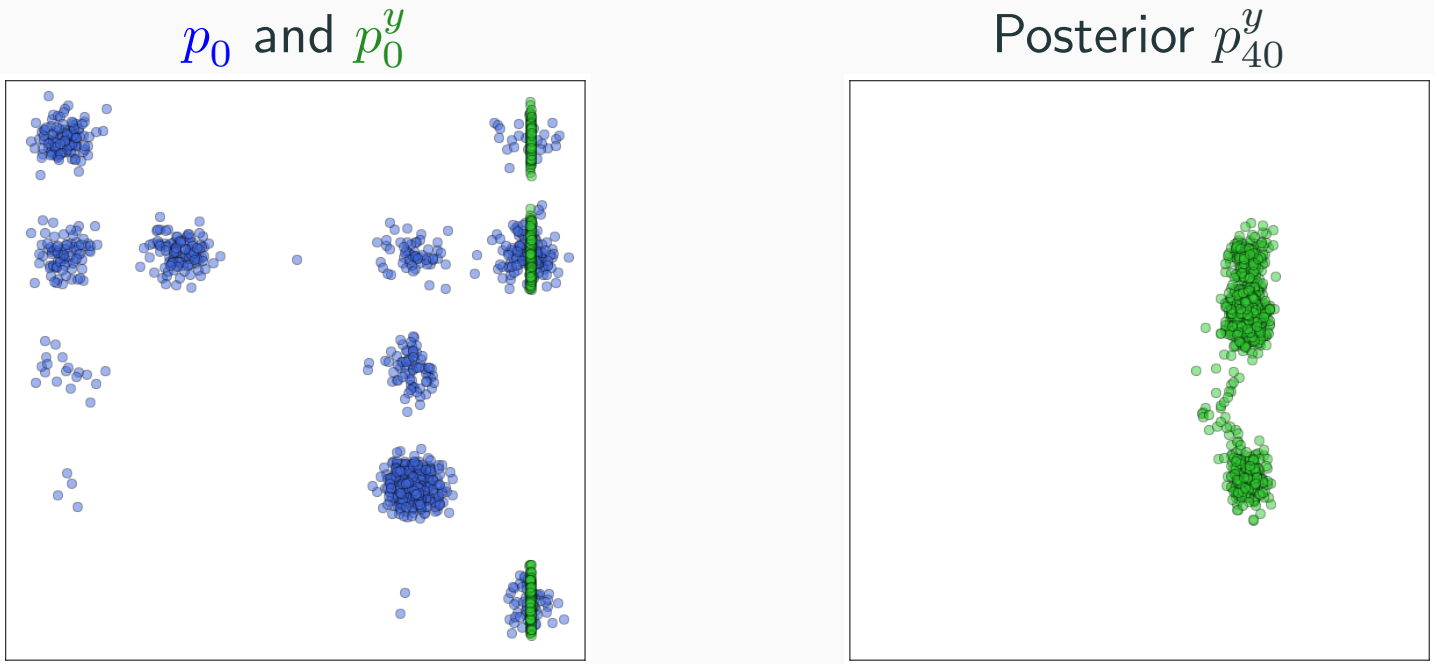


Figure 12: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

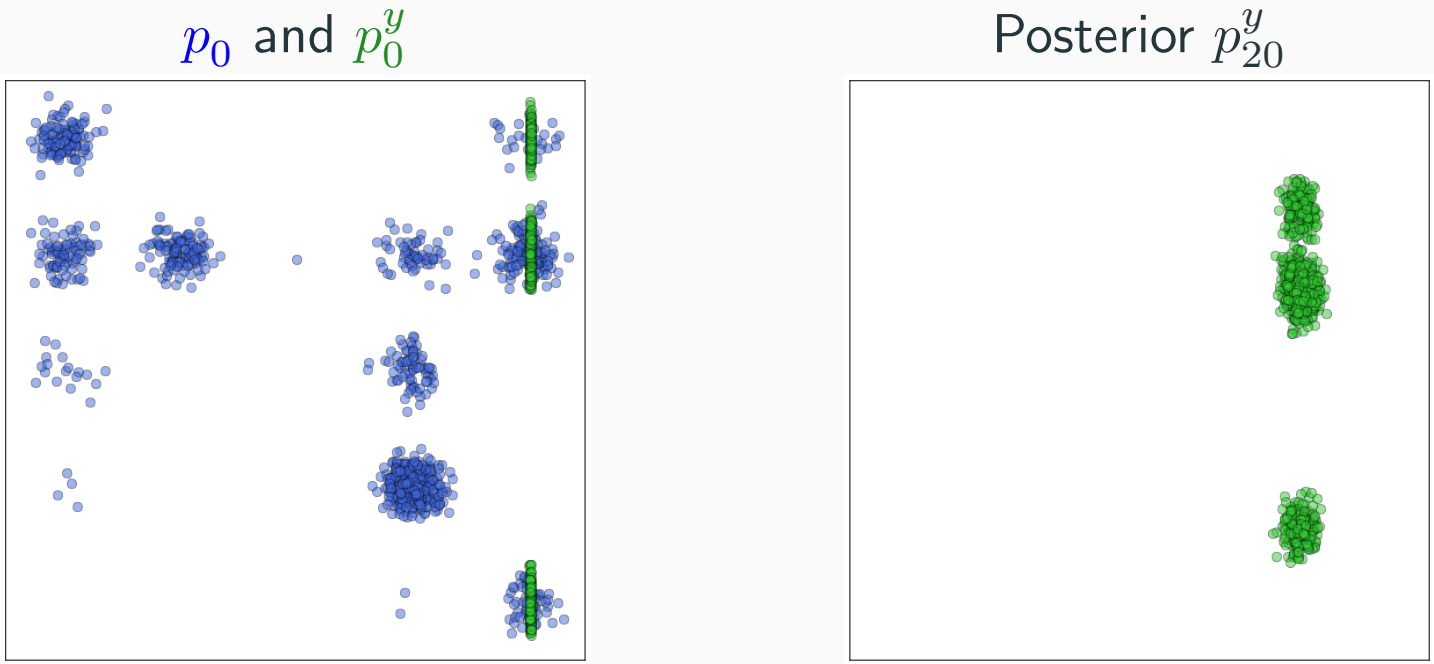


Figure 13: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

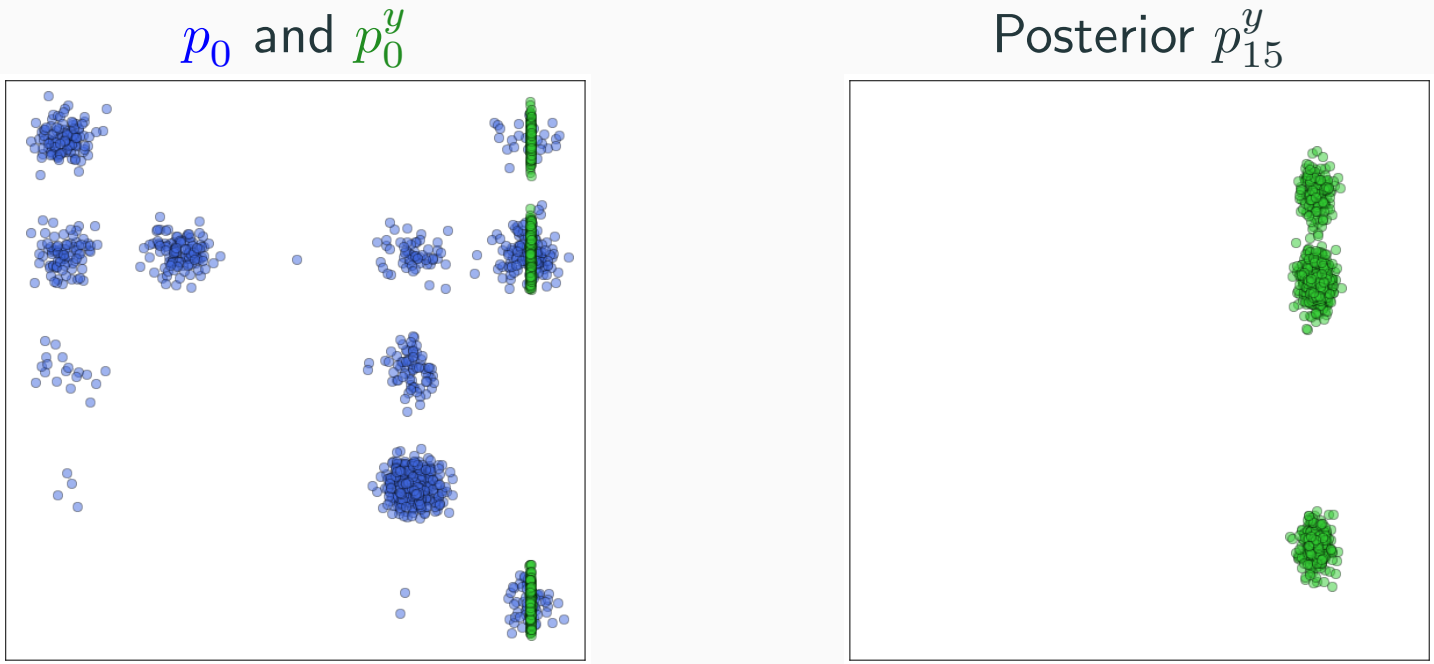


Figure 14: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

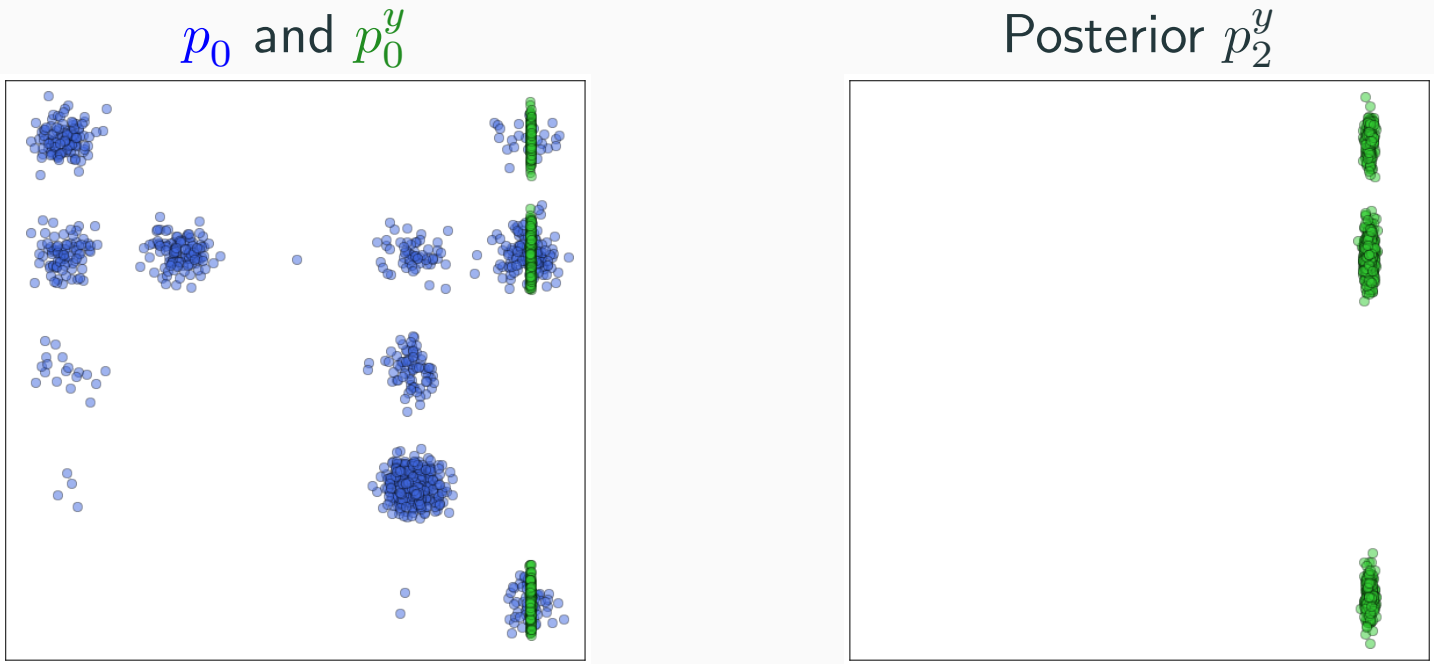


Figure 15: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

Illustration

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

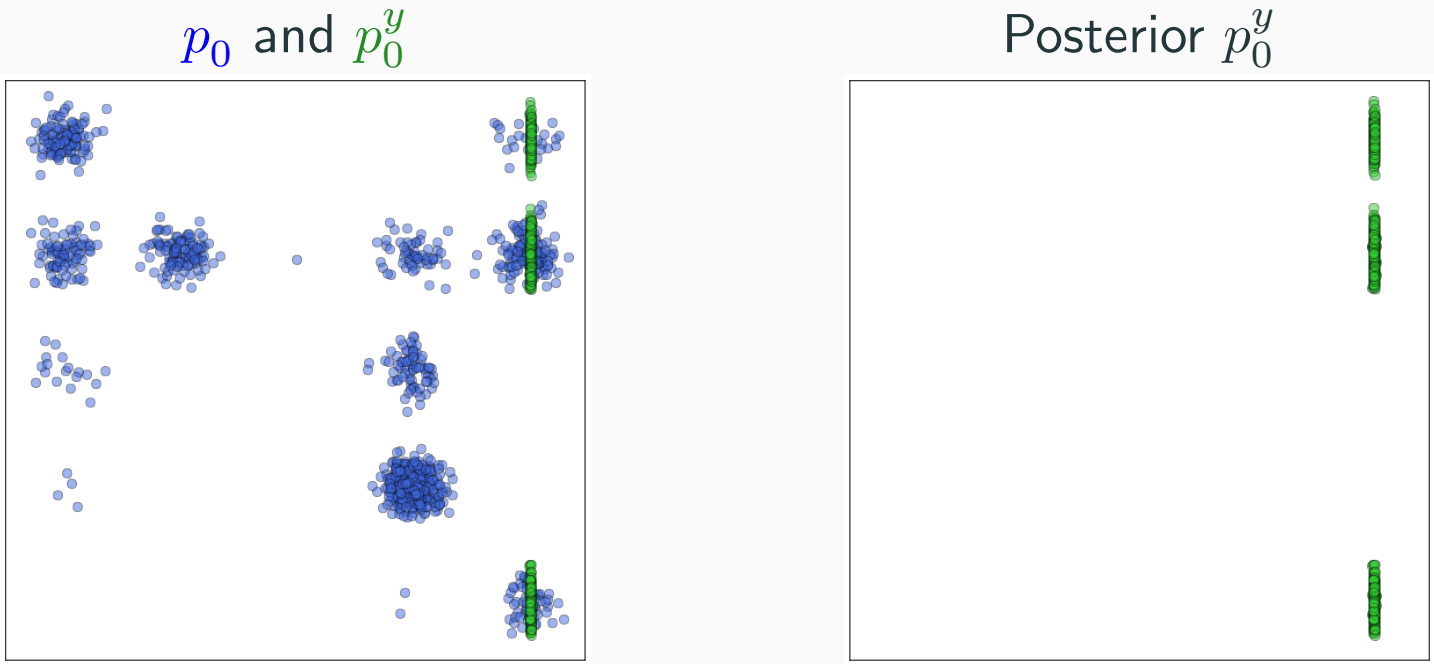


Figure 16: Left plot: samples from the prior p_0 and posterior p_0^y. **Right plot:** samples from the posterior proposals p_k^y for time steps ranging from $n := 500$ to 0.

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

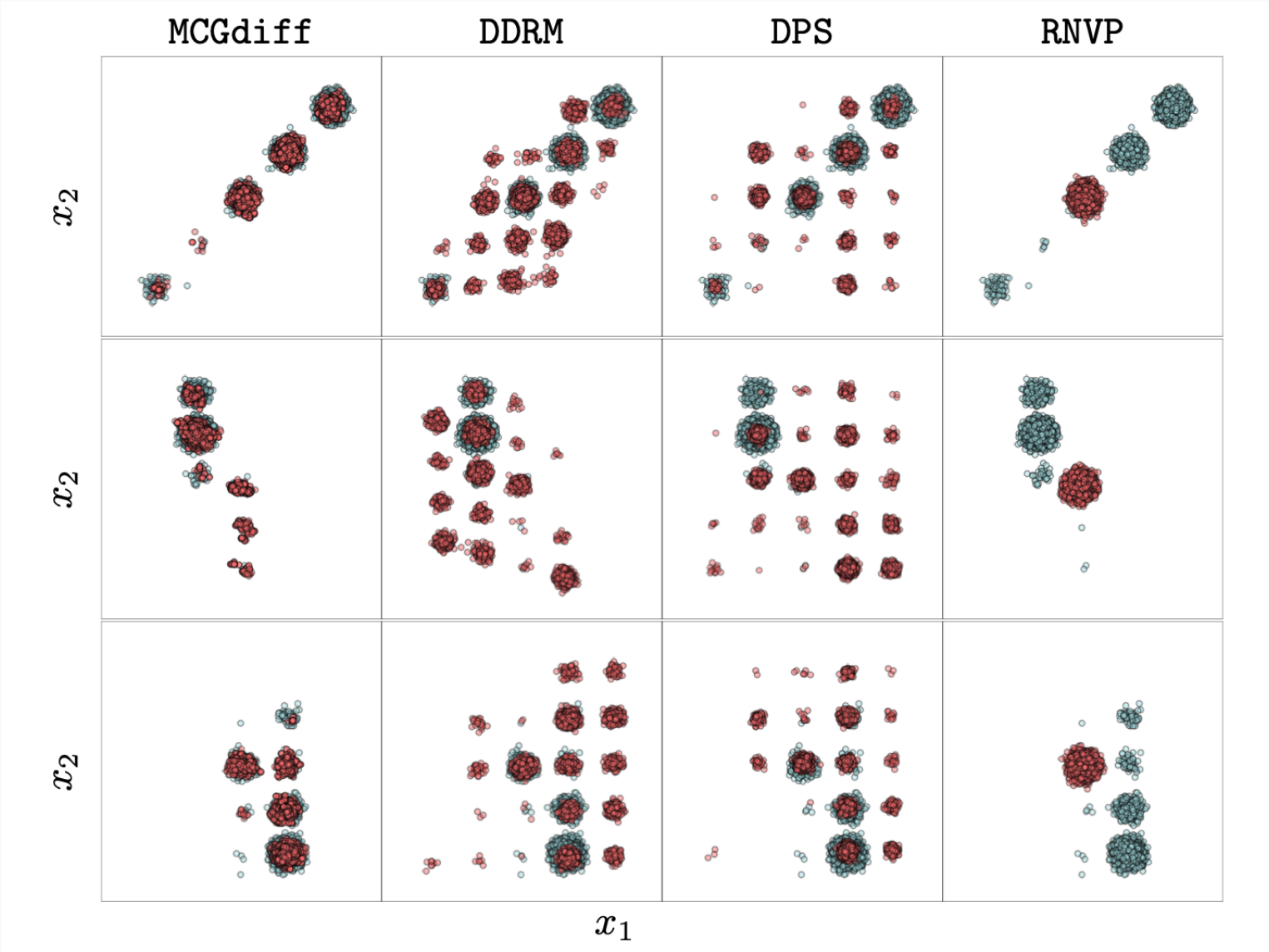
d	d_y	MCGdiff	DDRM	DPS	RNVP
80	1	**1.39 ± 0.45**	5.64 ± 1.10	4.98 ± 1.14	6.86 ± 0.88
80	2	**0.67 ± 0.24**	7.07 ± 1.35	5.10 ± 1.23	7.79 ± 1.50
80	4	**0.28 ± 0.14**	7.81 ± 1.48	4.28 ± 1.26	7.95 ± 1.61
800	1	**2.40 ± 1.00**	7.44 ± 1.15	6.49 ± 1.16	7.74 ± 1.34
800	2	**1.31 ± 0.60**	8.95 ± 1.12	6.88 ± 1.01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



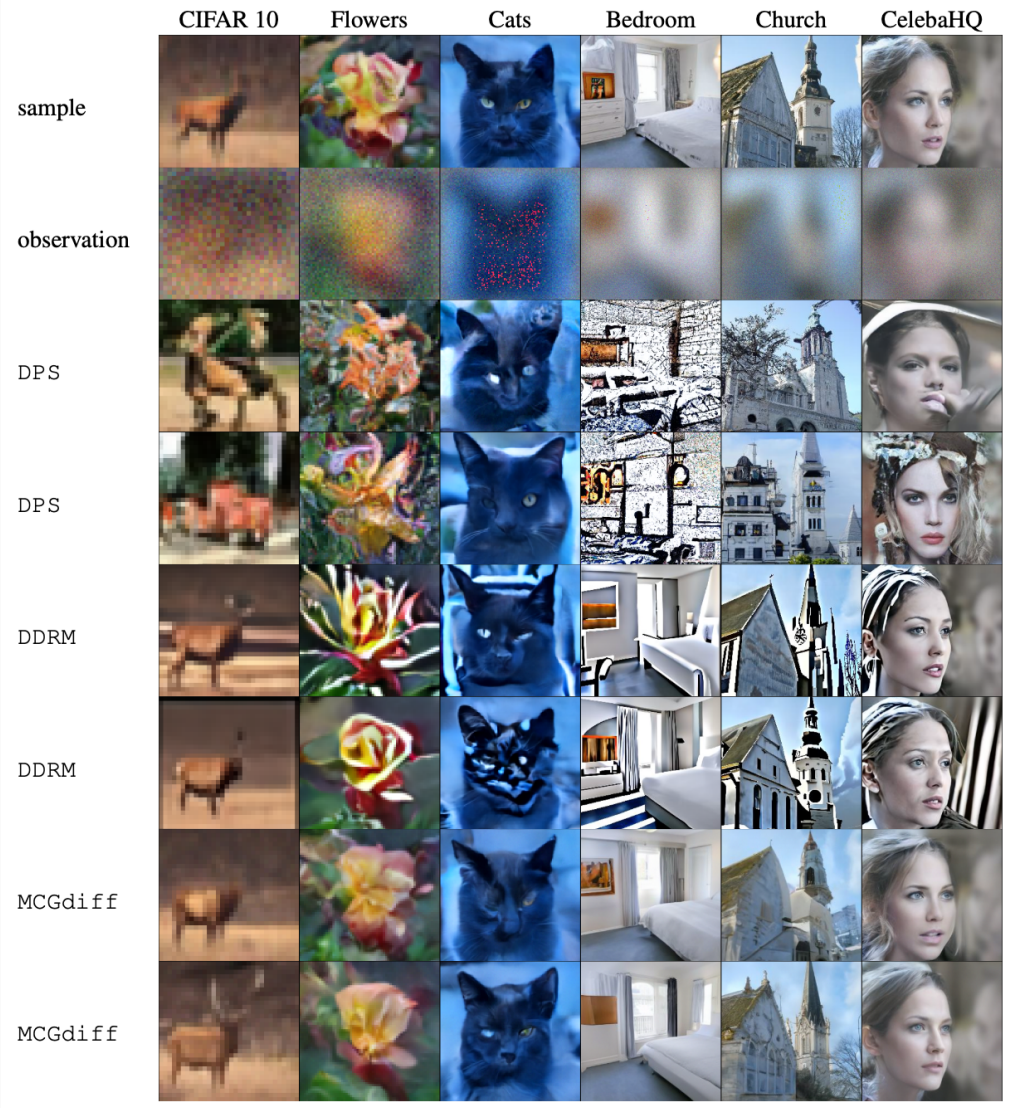
Imaging experiments

- $\rightsquigarrow$ 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

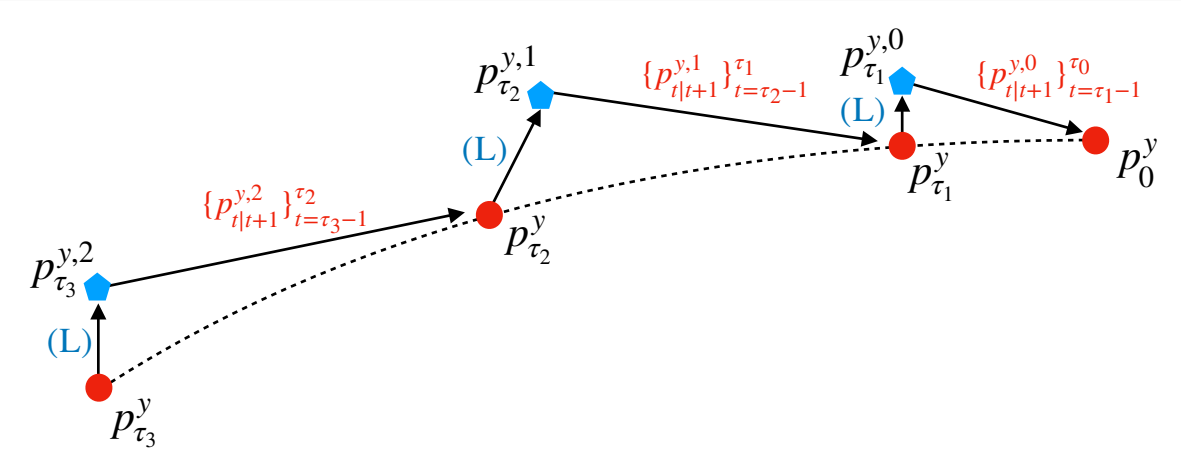


Figure 18: Illustration of idealized DCPS.

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

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

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 $s^{y,\ell}_{j|j+1} \in \mathbb{R}^{d_x}$,

$$\mathsf{KL}(r^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1}) \,\|\, \hat{p}^{y,\ell}_{j|j+1}(\cdot|X^{y,\ell}_{j+1}))$$

$$= -\mathbb{E}\big[\log \hat{\beta}^{y,\ell}_{k_\ell|j}(\mu^{y,\ell}_{j|j+1} + \mathrm{diag}(\mathrm{e}^{s^{y,\ell}_{j|j+1}})Z)\big] + \frac{\|\mu^{y,\ell}_{j|j+1} - \mu_{j|j+1}(X^{y,\ell}_{j+1})\|^2}{2\sigma^2_{m|m+1}}$$

$$- \frac{1}{2}\sum_{i=1}^{d_x}\left(s^{y,\ell}_{j|j+1,i} - \frac{\mathrm{e}^{s^{y,\ell}_{j|j+1,i}}}{\sigma^2_{m|m+1}}\right),$$

- 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 $(X^{y,\ell}_j)_{j=k_{\ell+1}}^{k_\ell}$: 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.

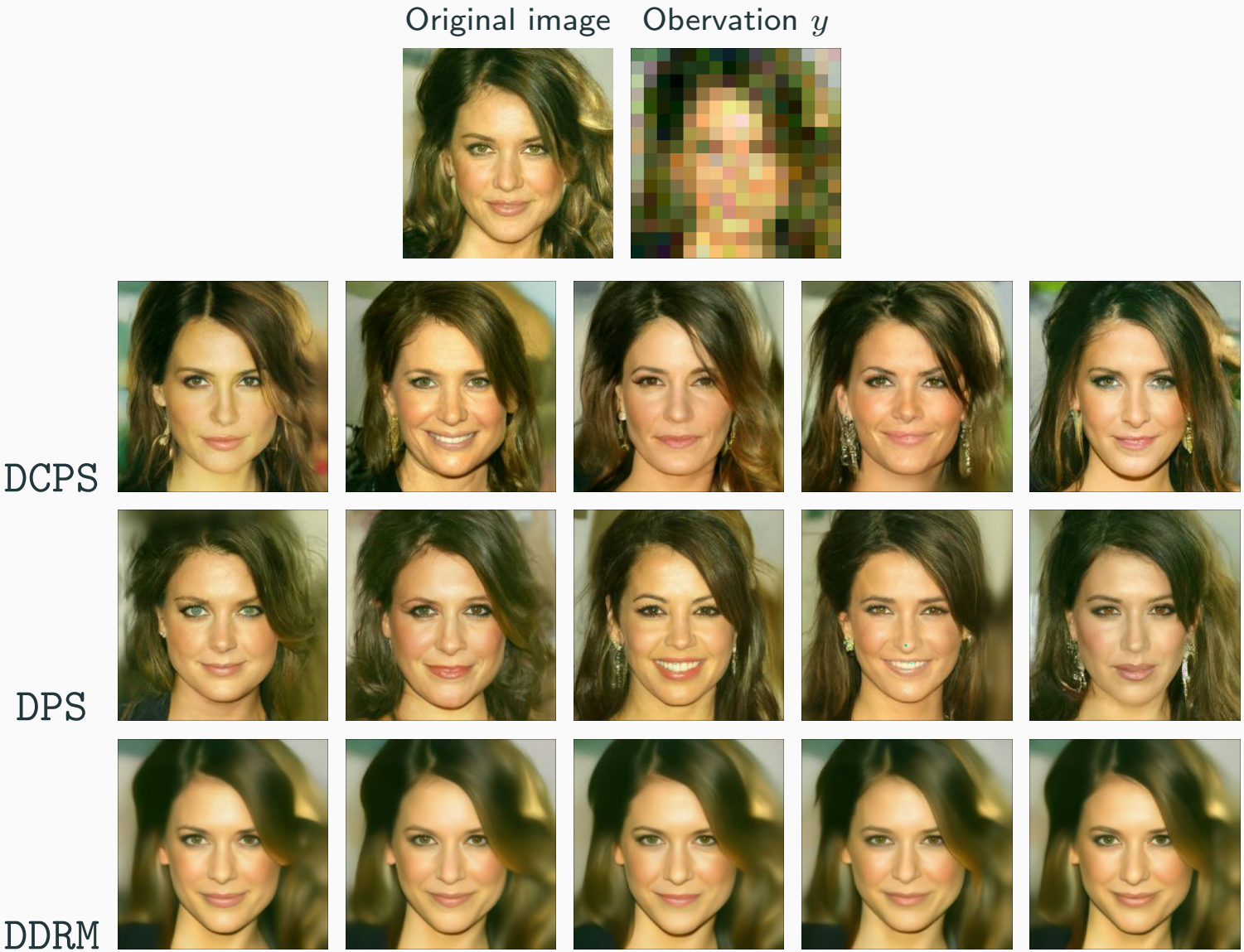
Toy experiments

- Same 25 Gaussian mixture example.
- M Langevin steps at the beginning of each block and $L = 4$.

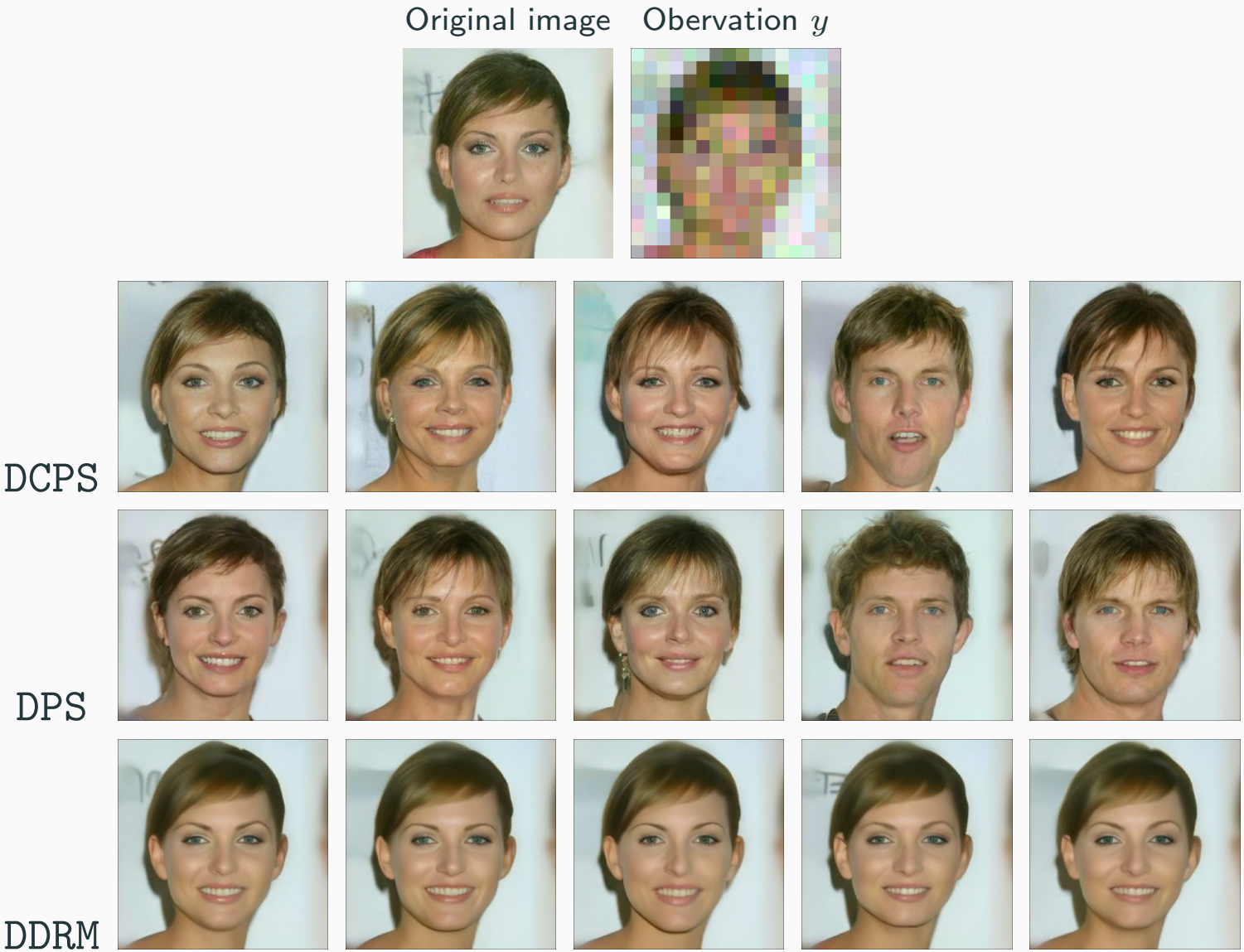
	$d_x = 10,\ d_y = 1$		$d_x = 100,\ d_y = 1$	
	SW	Δw	SW	Δw
`MCGDiff`	$2.25/2.69 \pm 2.07$	0.32 ± 0.20	$2.72/3.13 \pm 1.76$	0.42 ± 0.19
`DPS`	$3.12/5.64 \pm 8.45$	0.20 ± 0.12	$4.29/4.93 \pm 4.85$	0.35 ± 0.25
`DDRM`	$2.66/3.06 \pm 1.90$	0.36 ± 0.16	$5.97/6.26 \pm 2.33$	0.52 ± 0.19
$\texttt{DCPS}_{50}$	$1.95/2.70 \pm 2.28$	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 distance are shown in median/mean $\pm$ standard deviation format.

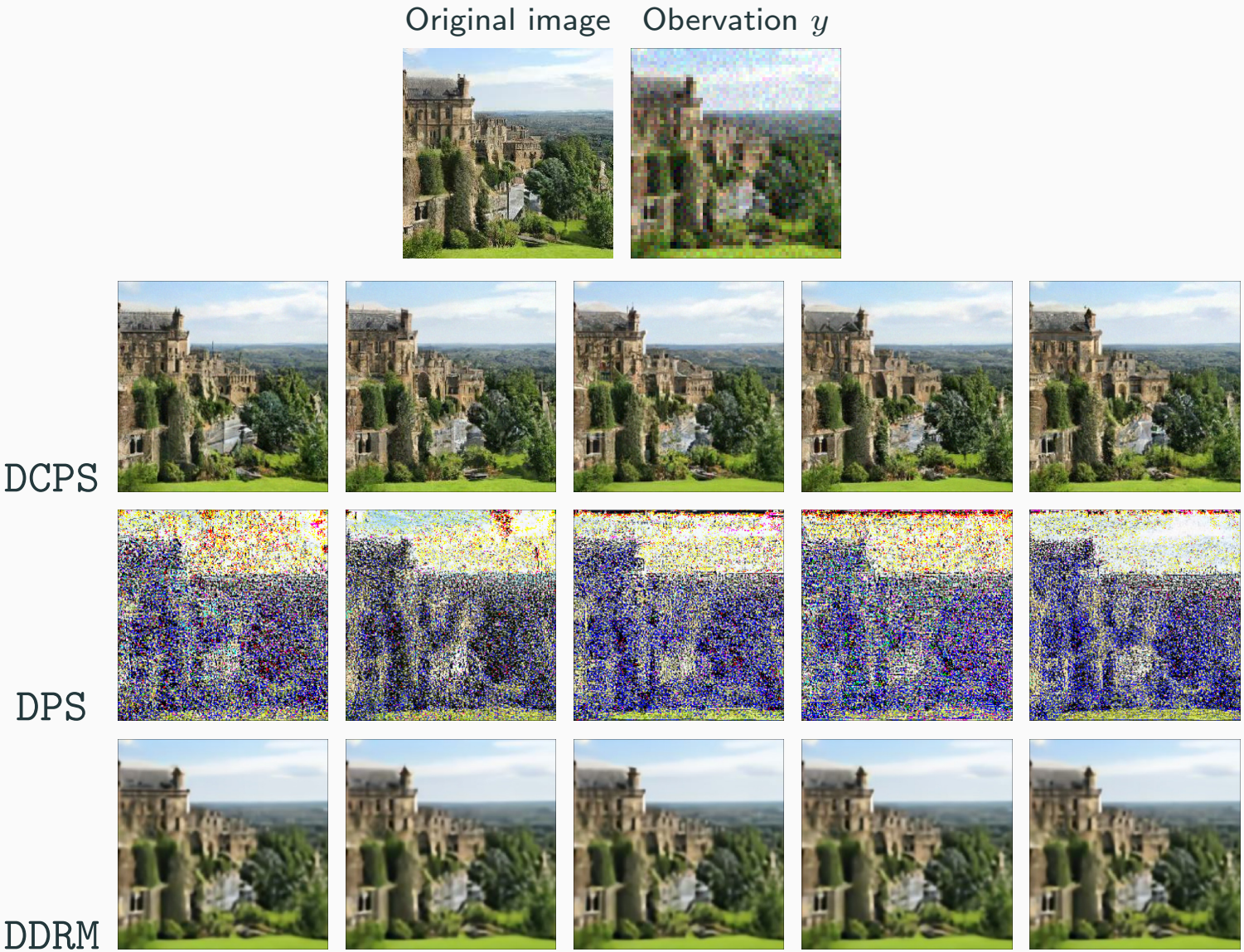
Super-resolution experiments



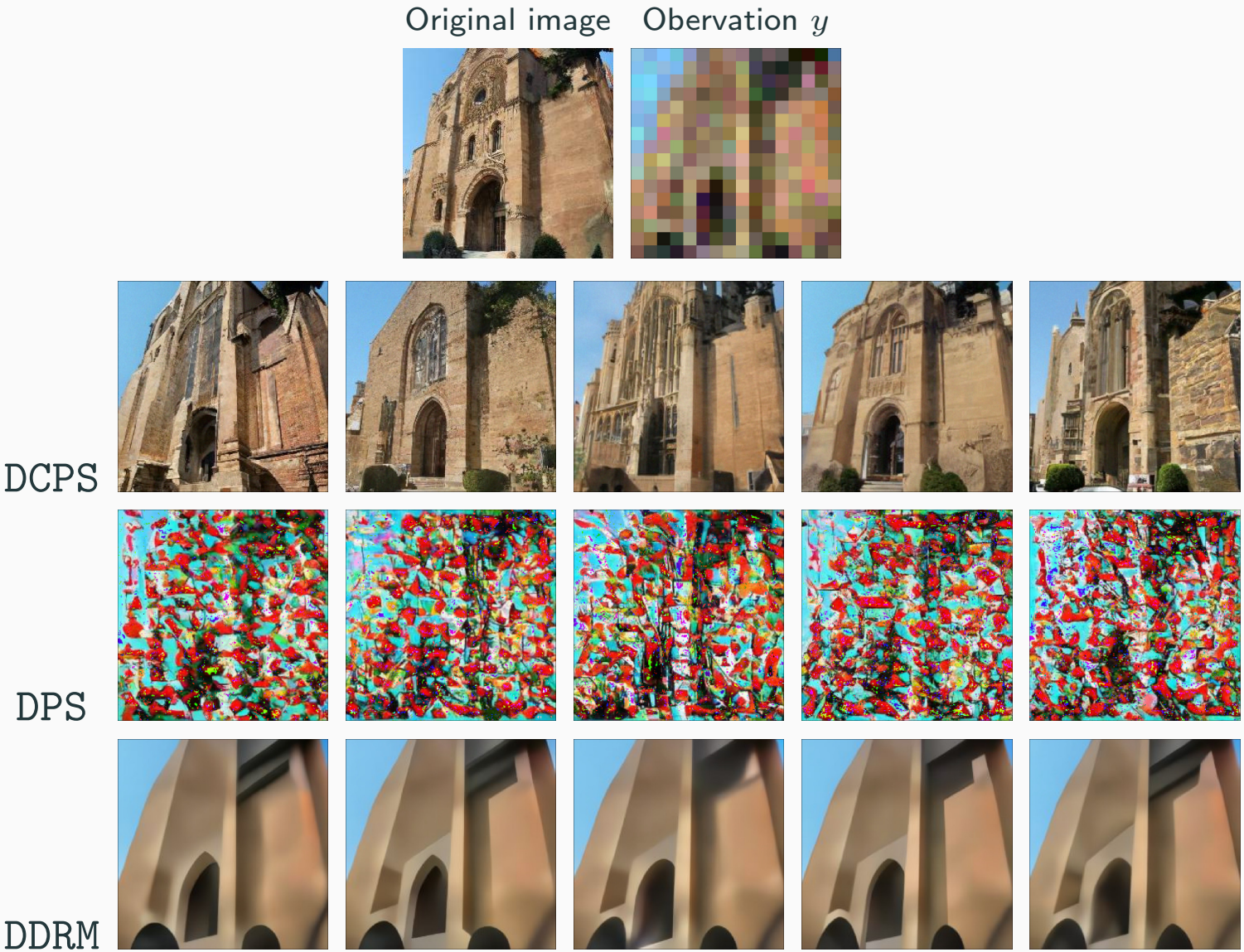
Super-resolution experiments



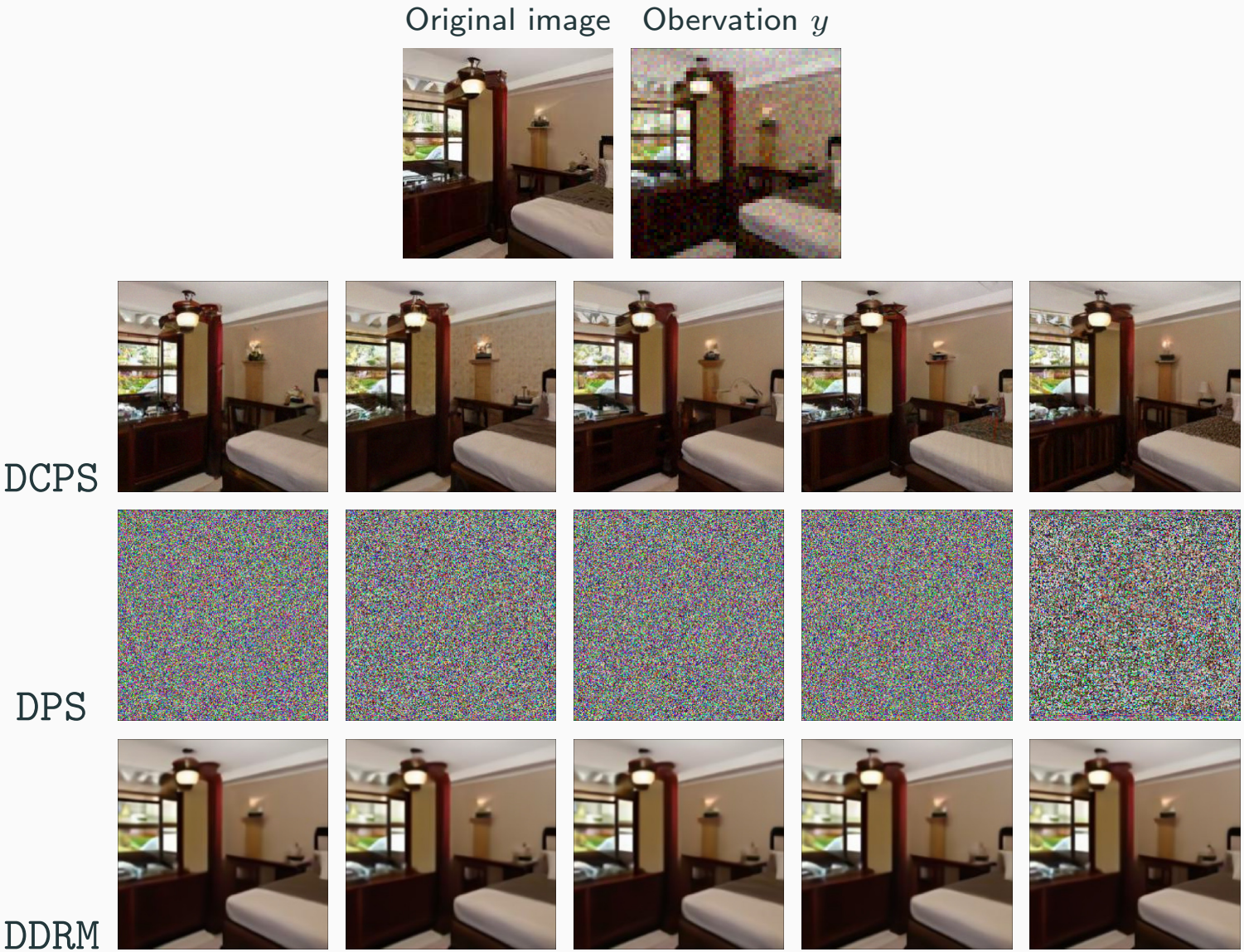
Super-resolution experiments



Super-resolution experiments

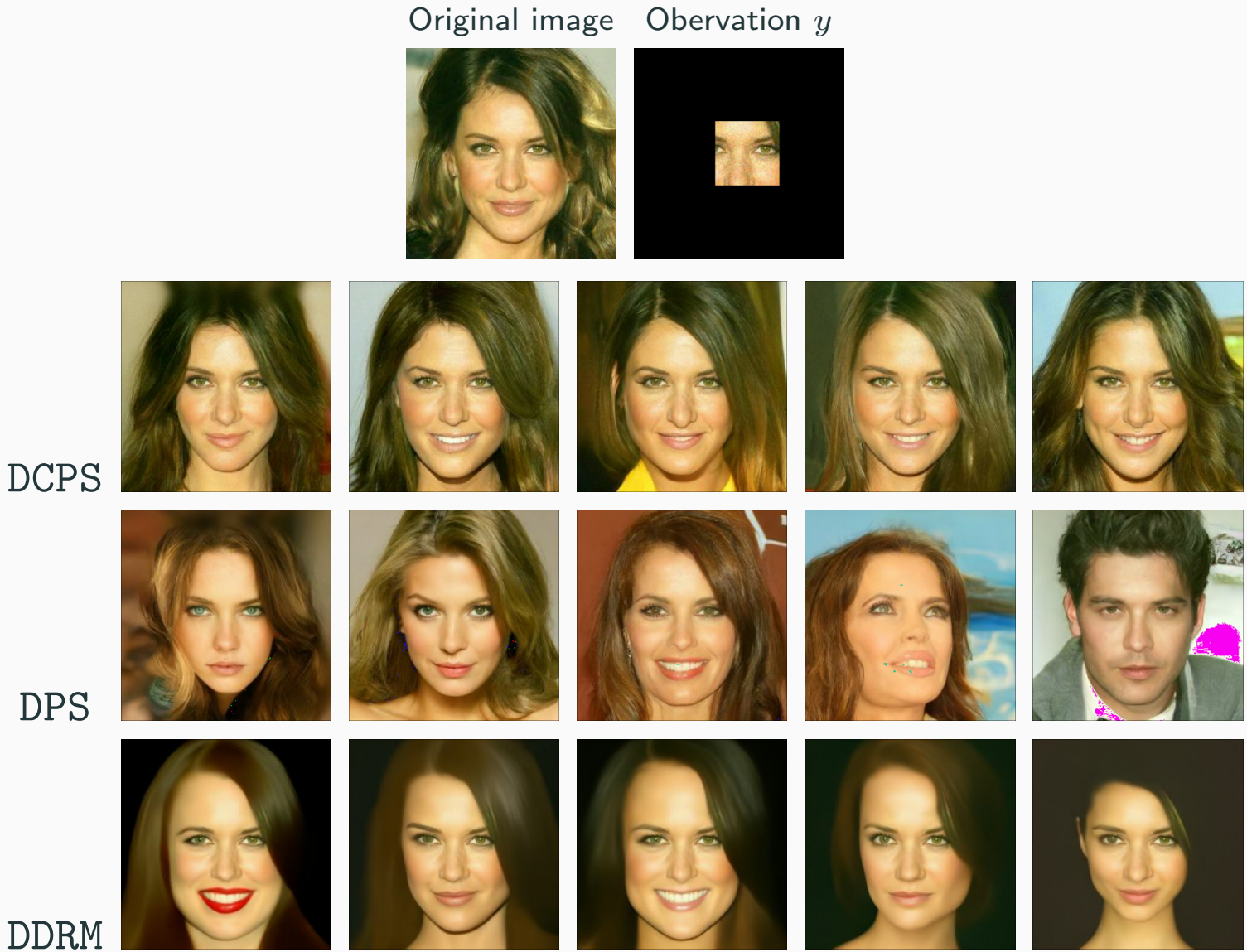


Super-resolution experiments



Super-resolution experiments

Inpainting and outpainting experiments



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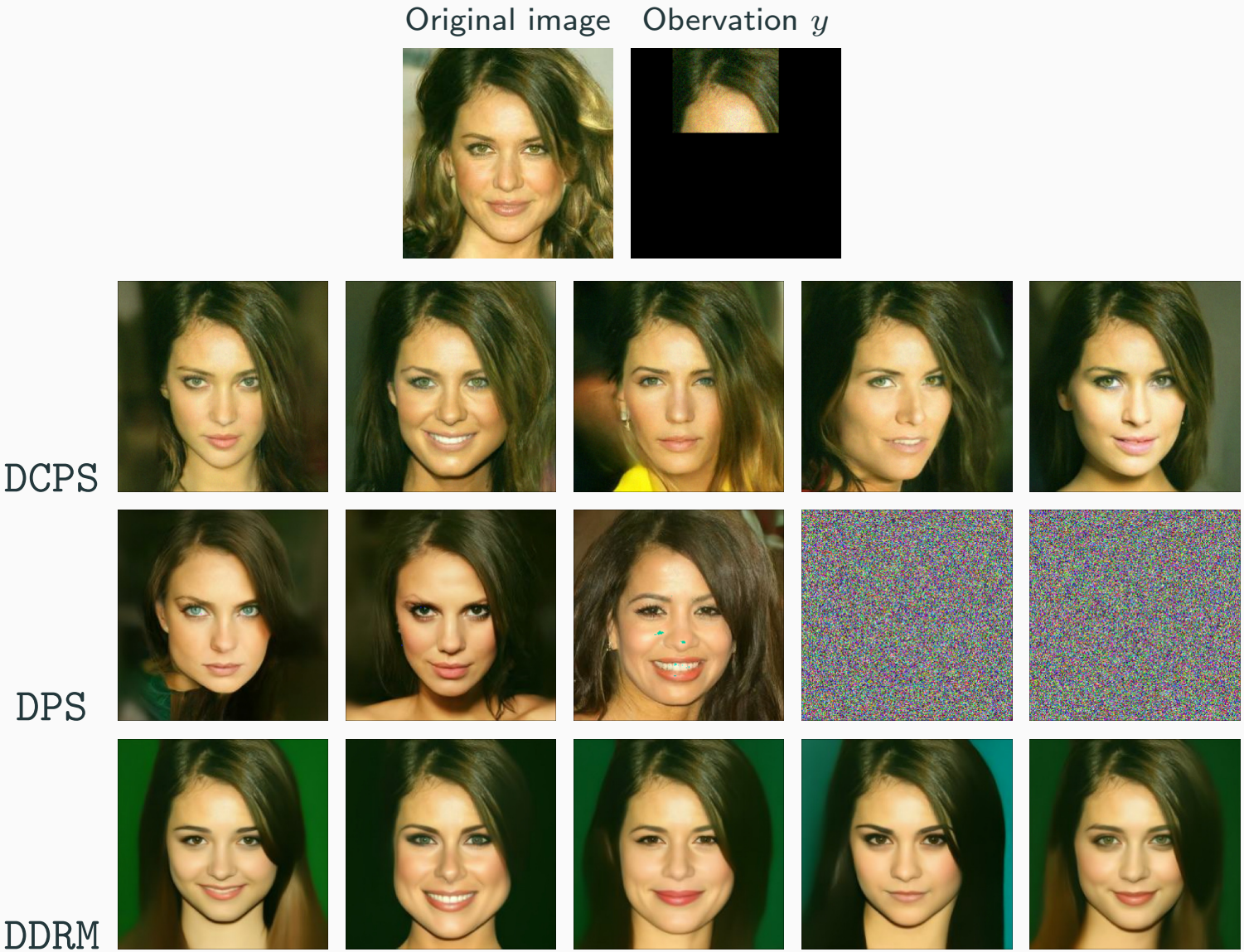
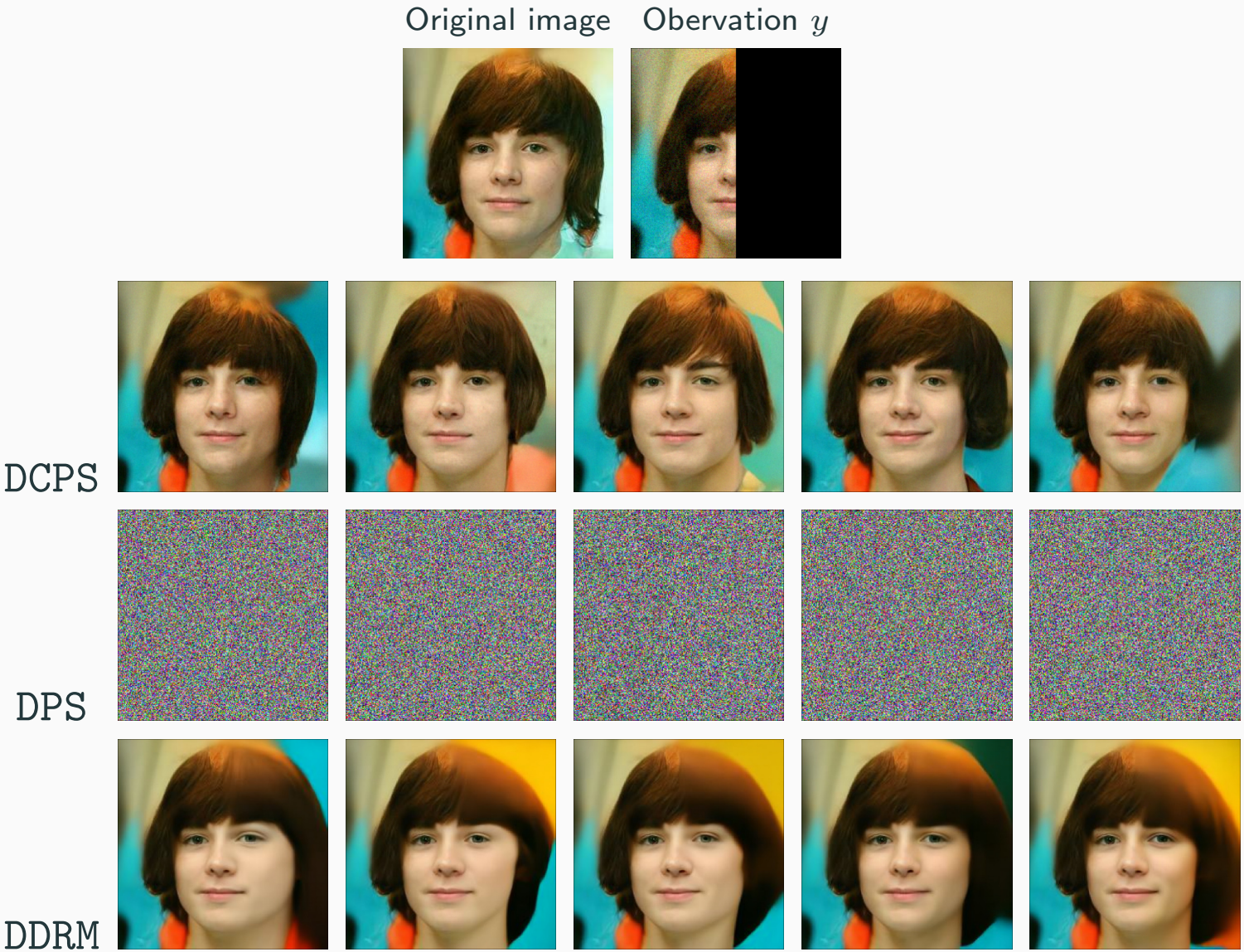


Inpainting and outpainting experiments



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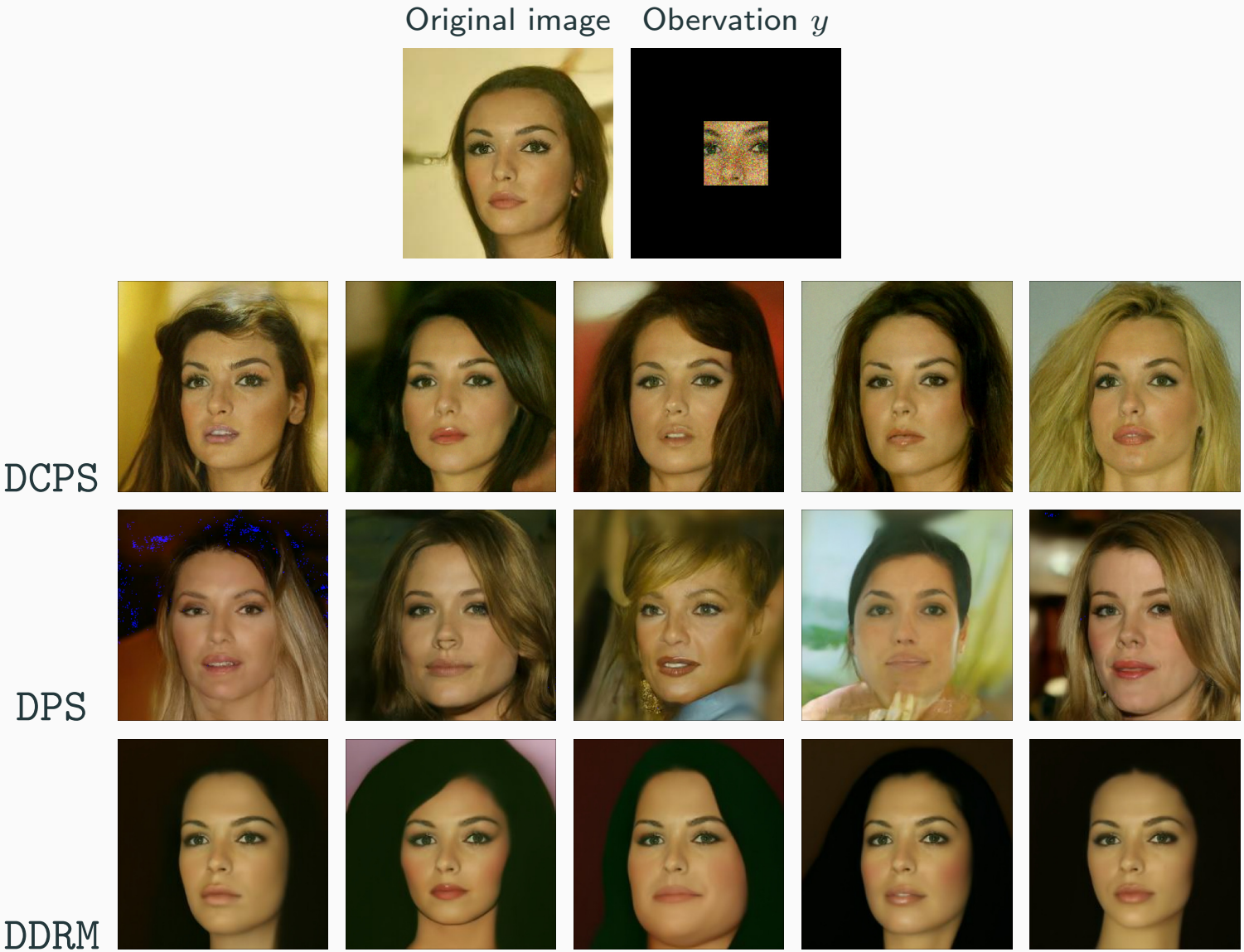

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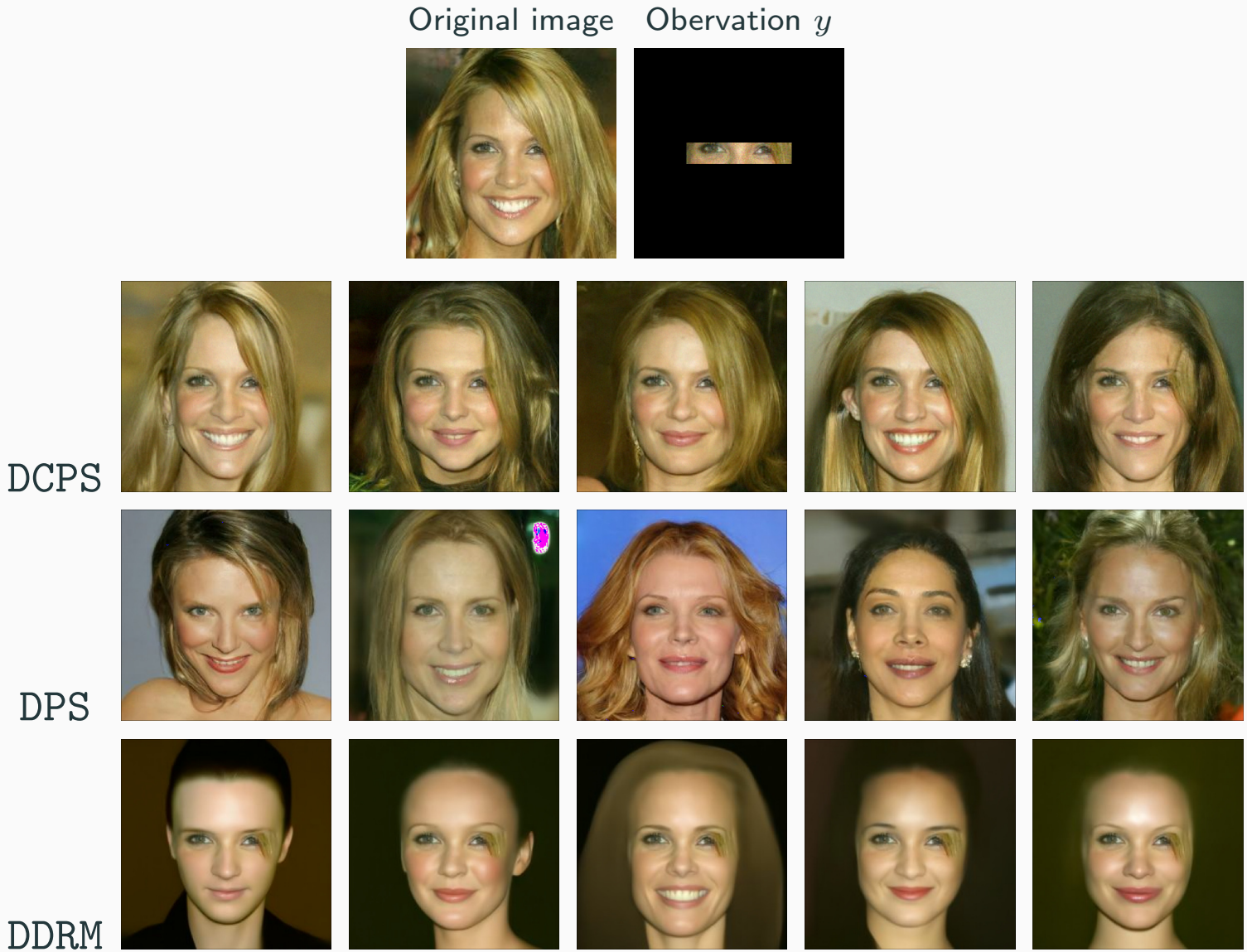
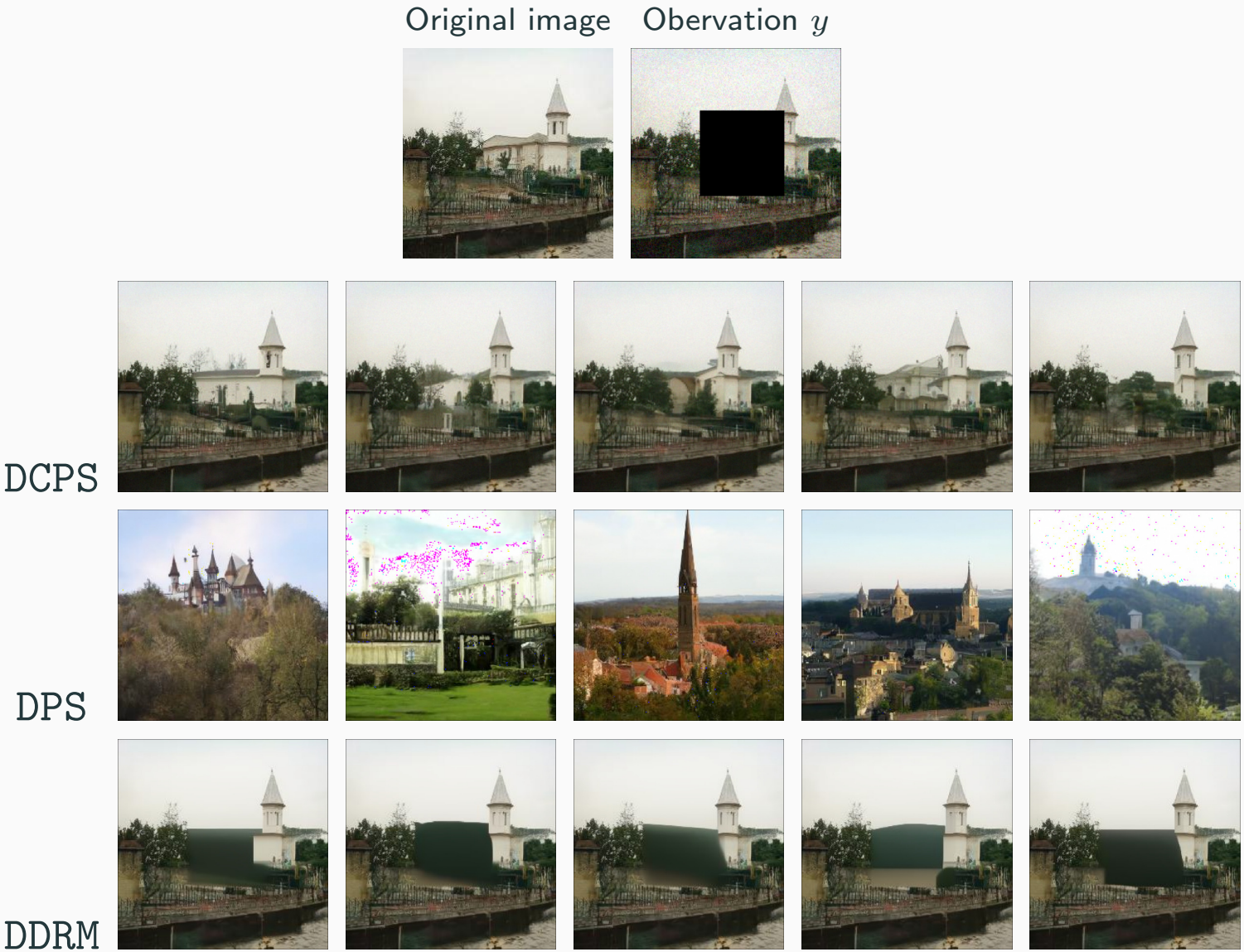


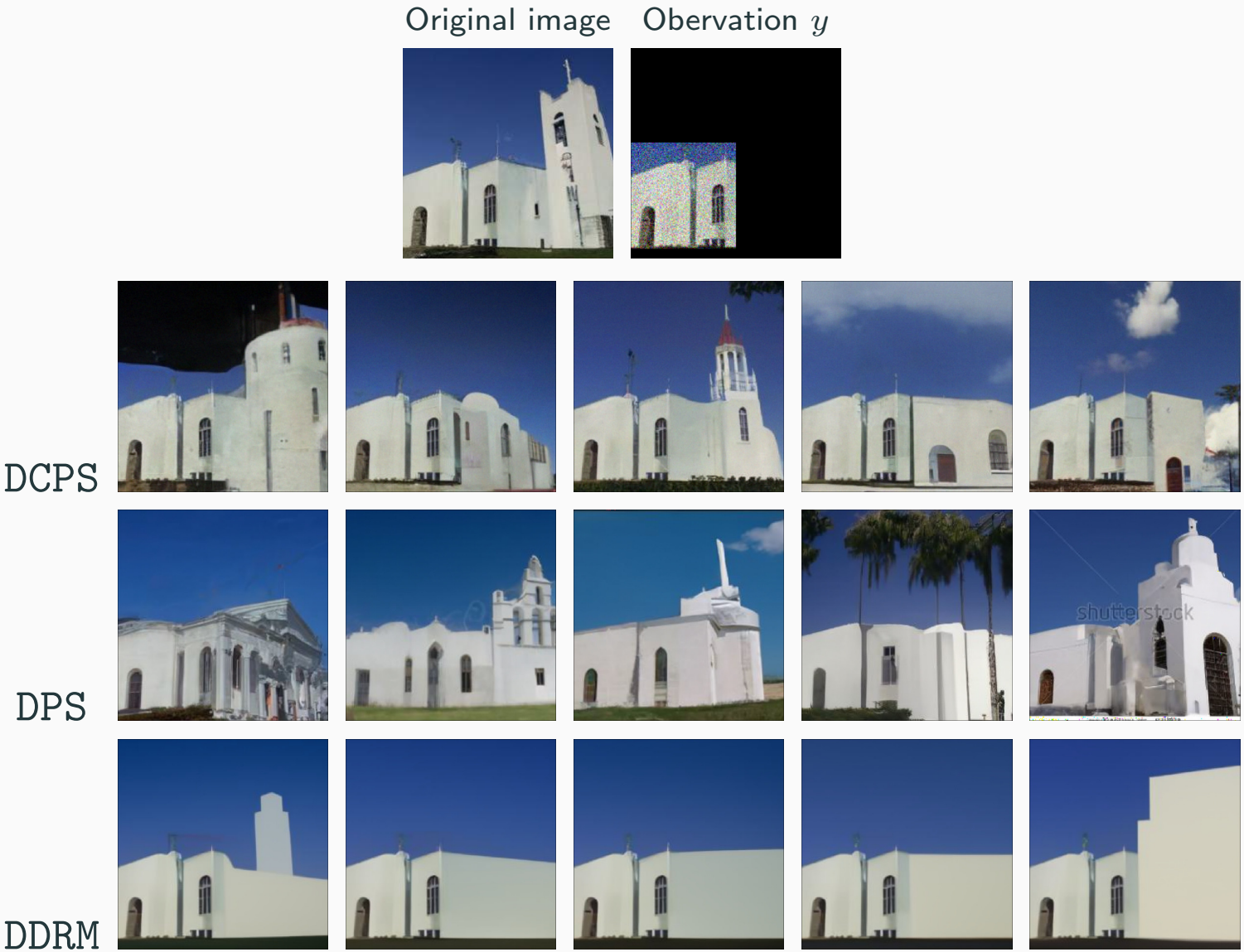
Inpainting and outpainting experiments

Inpainting and outpainting experiments



Inpainting and outpainting experiments

Inpainting and outpainting experiments



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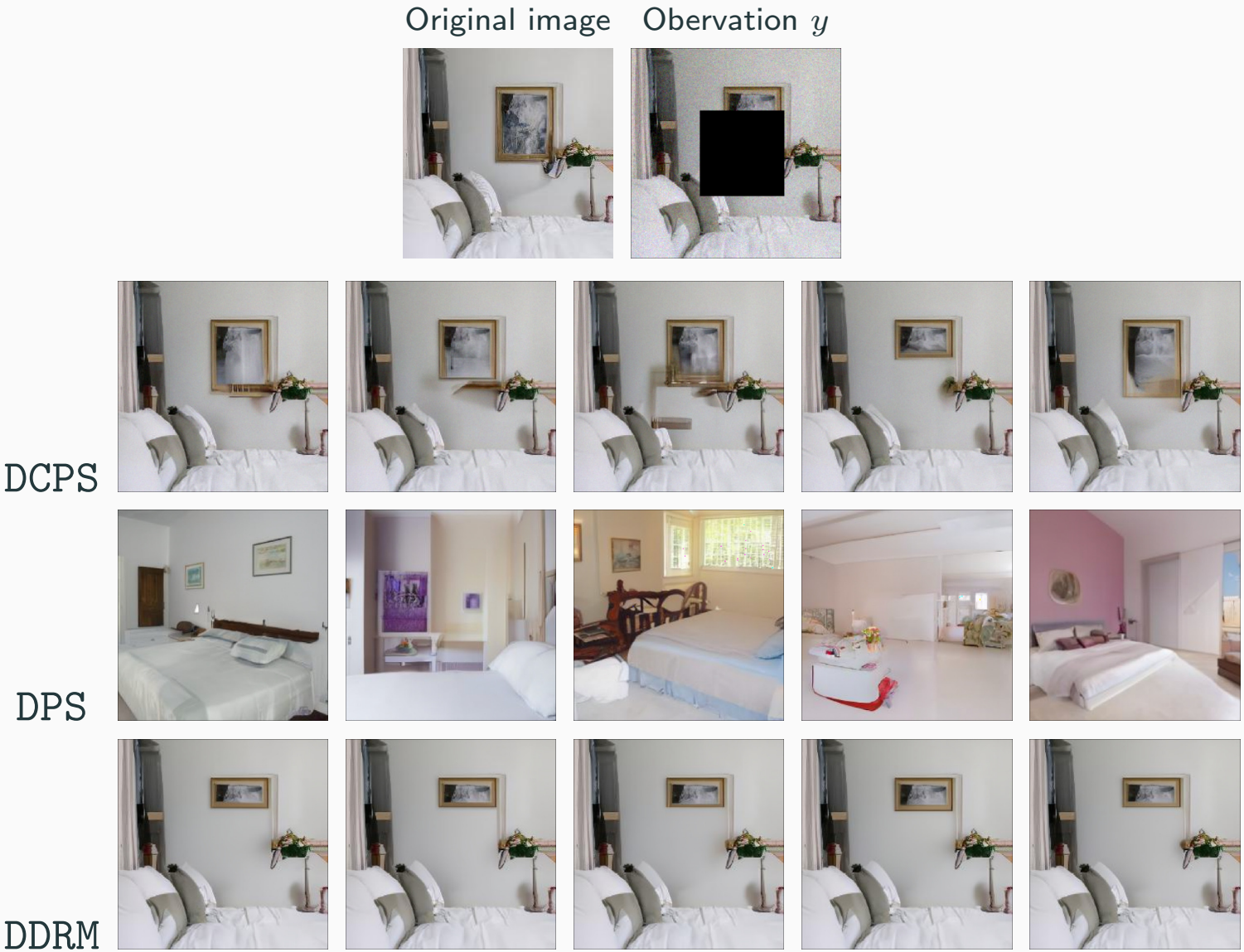
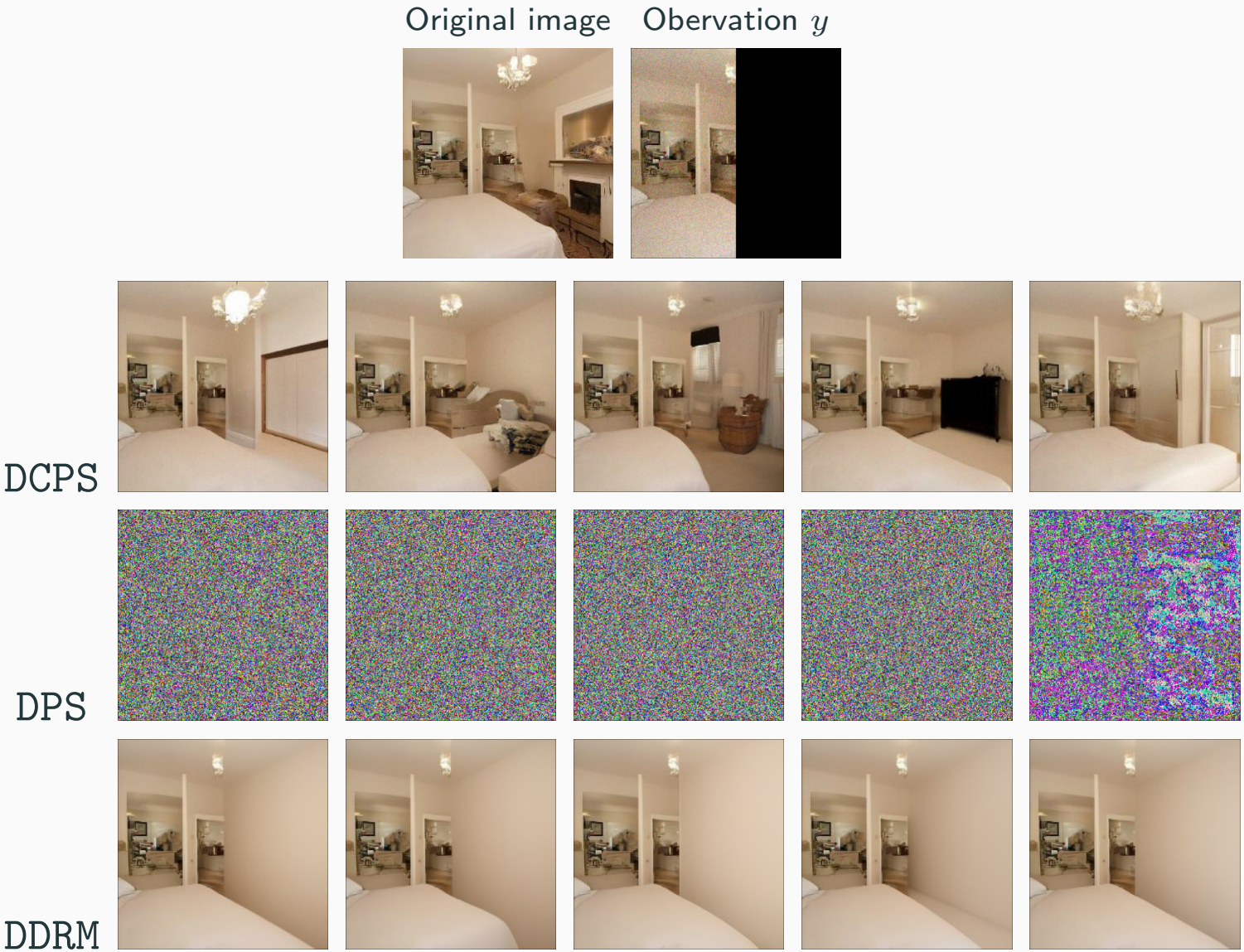
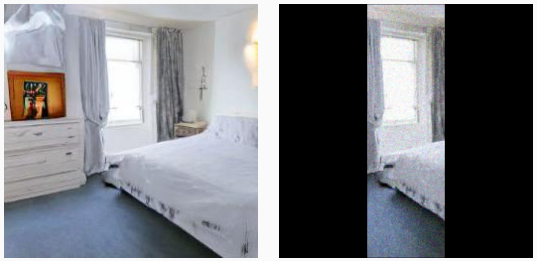


Inpainting and outpainting experiments

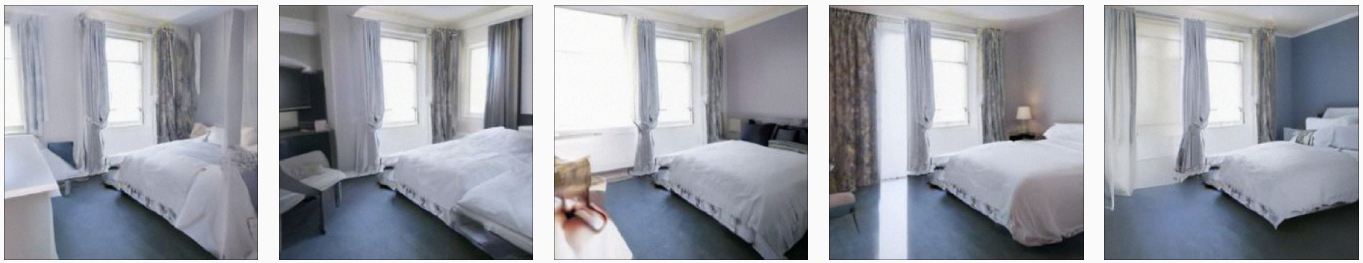


Inpainting and outpainting experiments

Original image | Obervation y

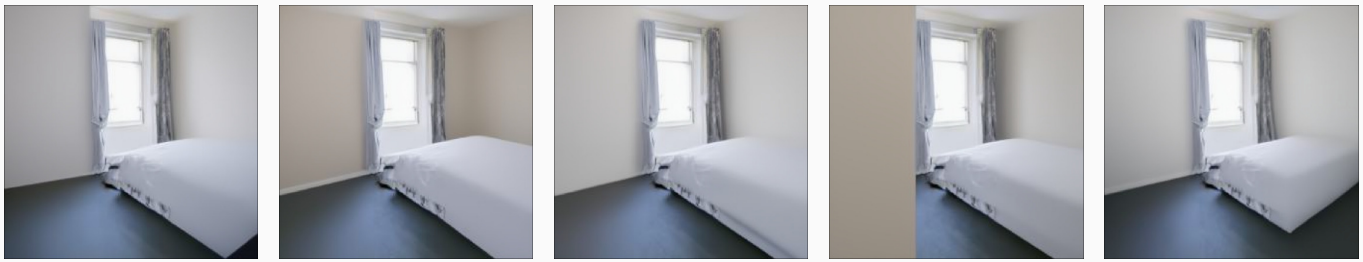


DCPS

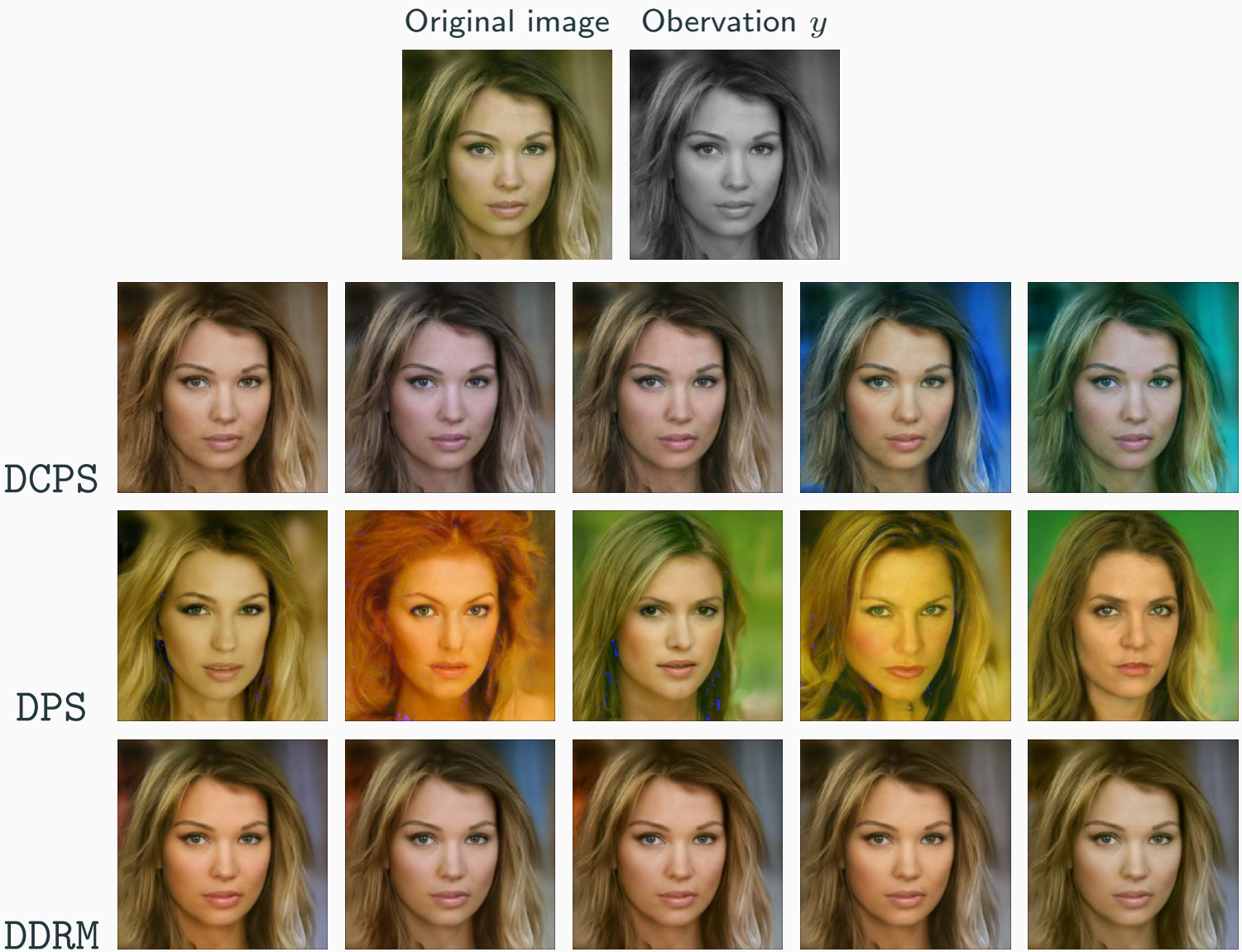


DPS

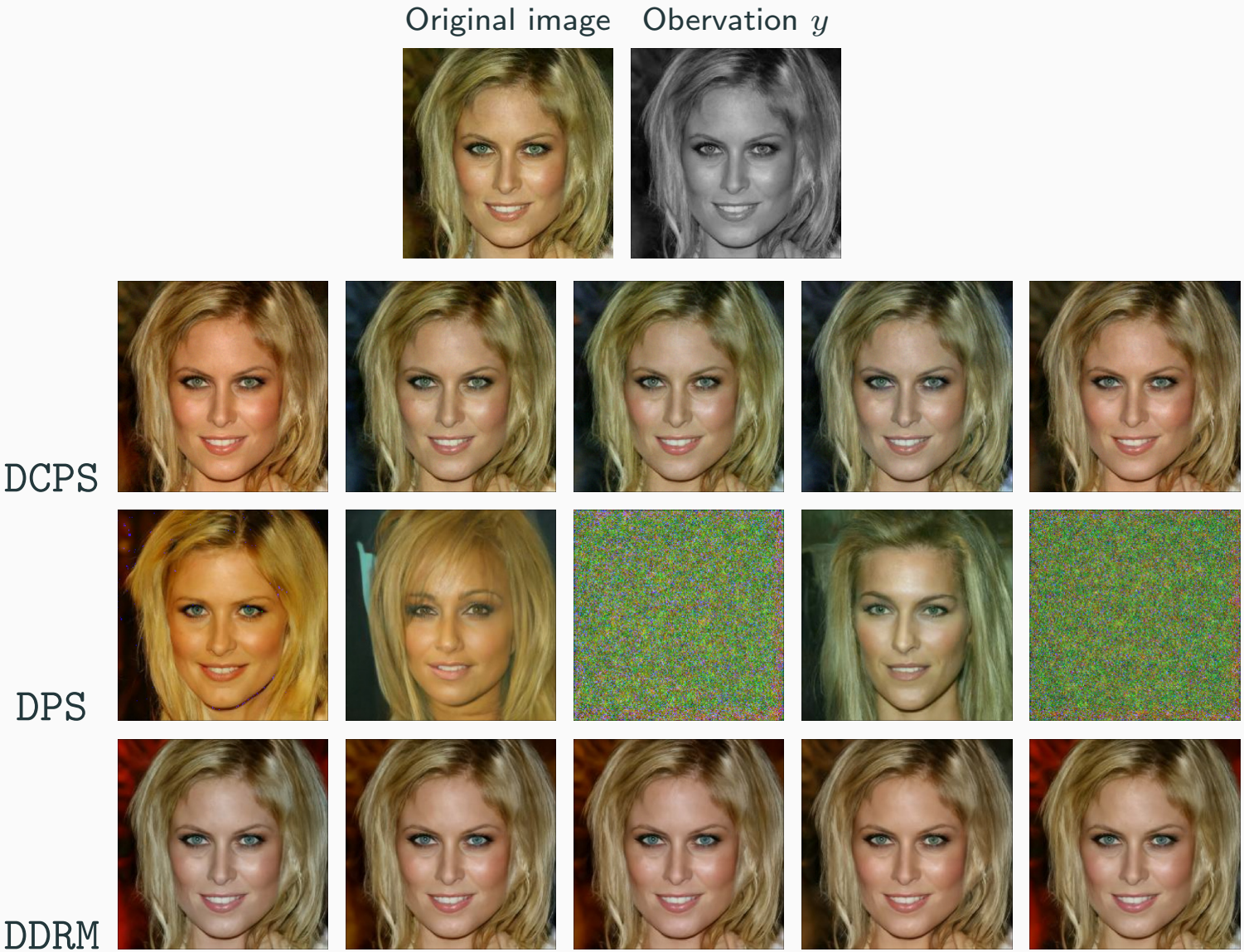
DDRM



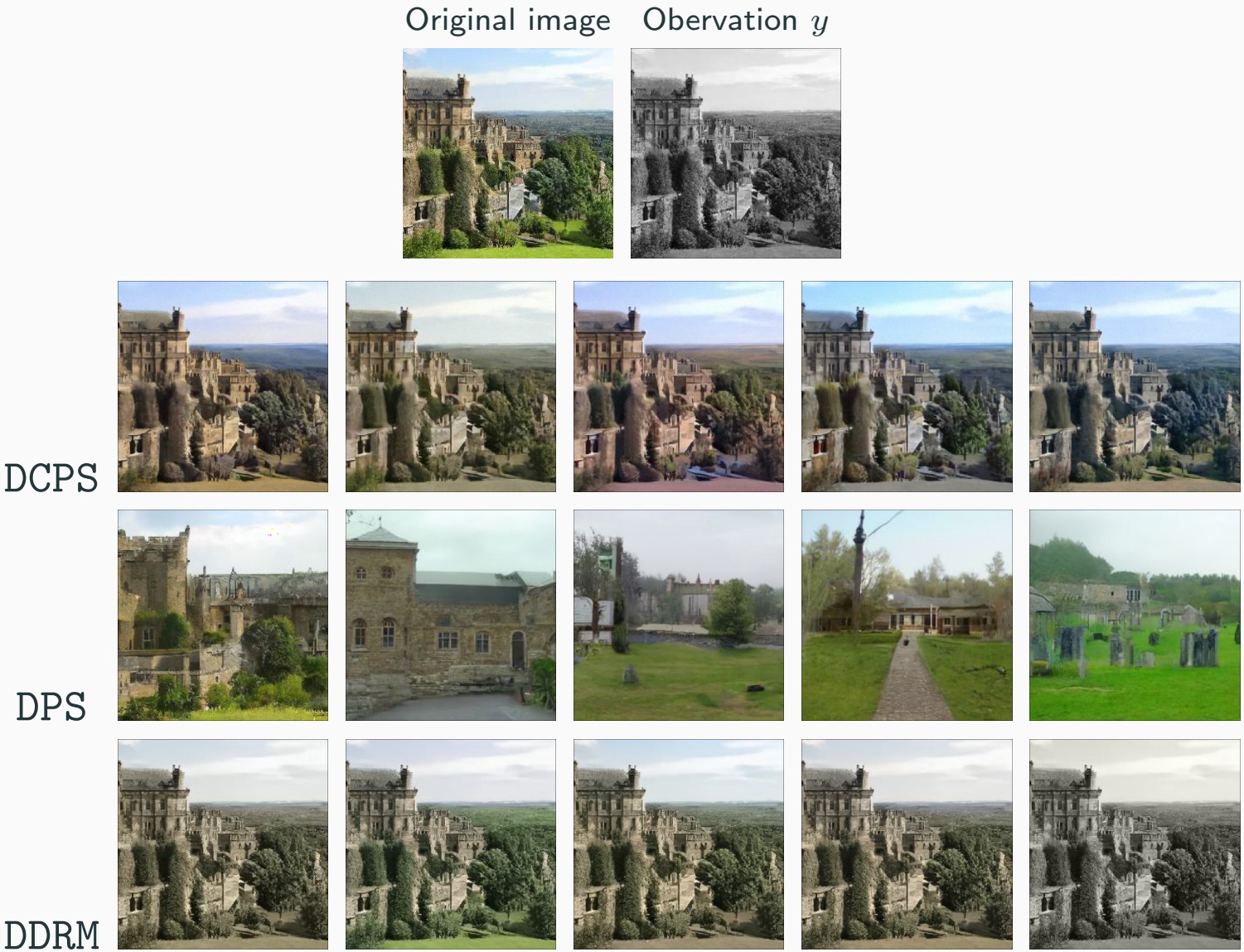
Colorization experiments



Colorization experiments



Colorization experiments



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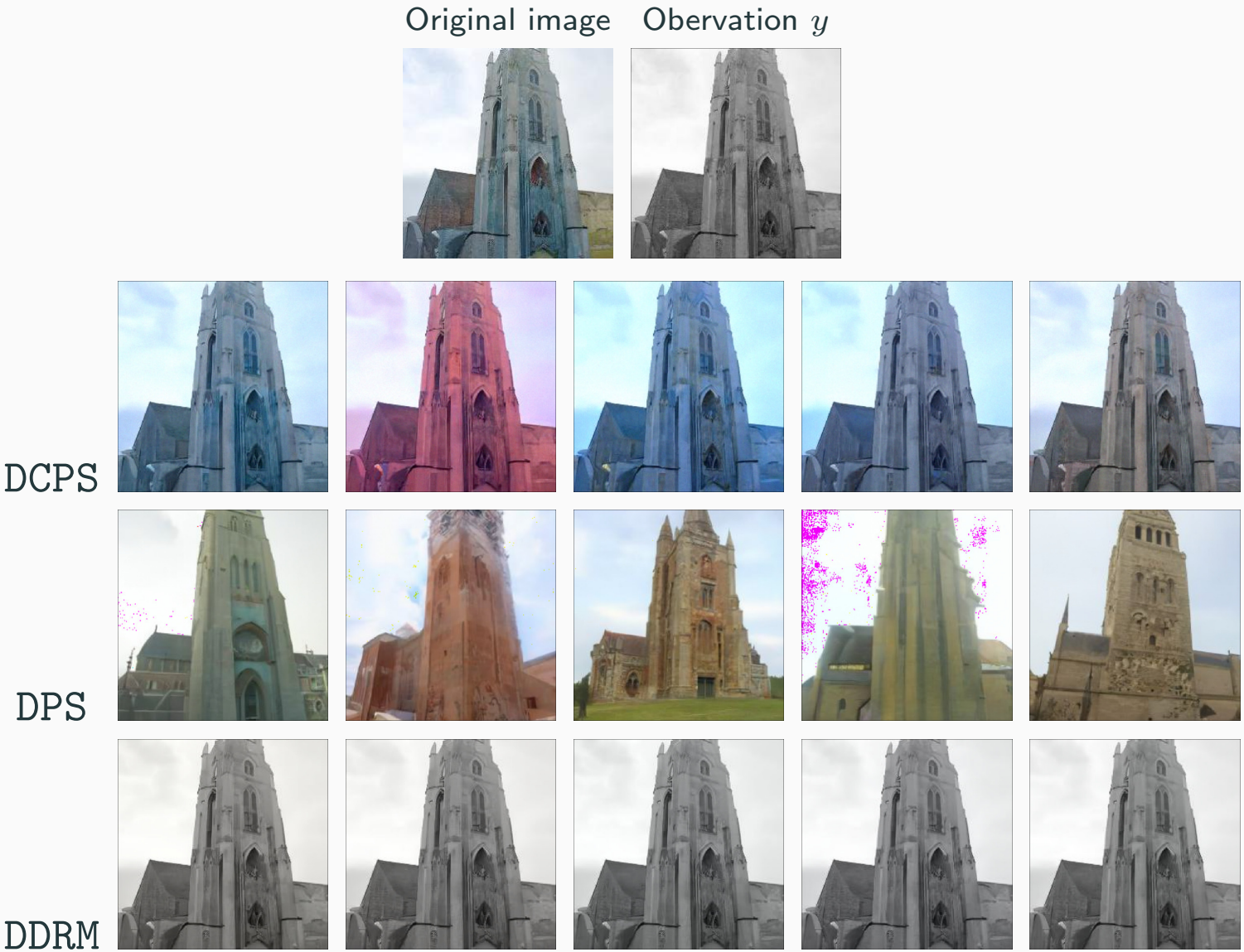
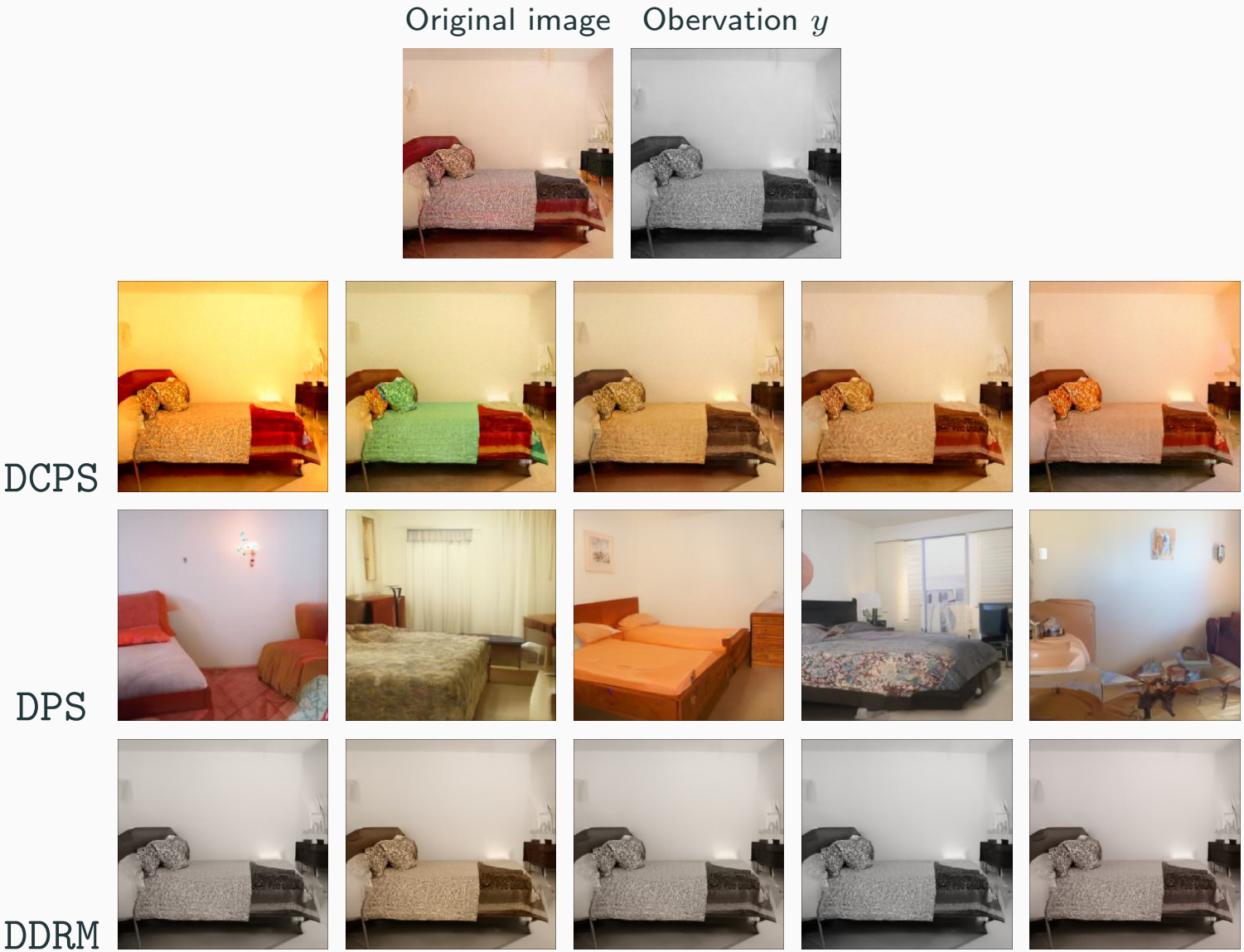


Colorization experiments



Thank you!

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