

# Monte Carlo sampling and deep generative models for Bayesian inference

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# Bayesian inference

**x**: unknown object of interest  
**y**: available data (observation)

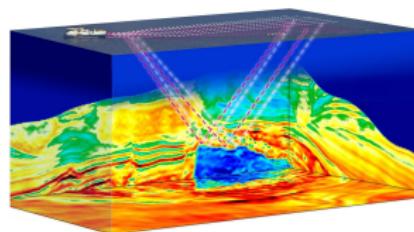
Update of prior information with available data<sup>1</sup>:

Prior $p(x)$	$\times$	Likelihood $p(y   x)$	$\rightarrow$	Posterior $p(x   y)$
↑ pre-observation knowledge		↑ acquisition process		↑ best guess

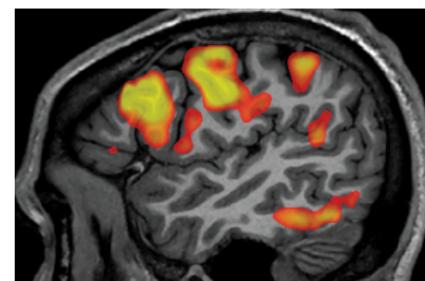
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<sup>1</sup>For complete review, see *Robert and Casella, 1999*

# Various applications



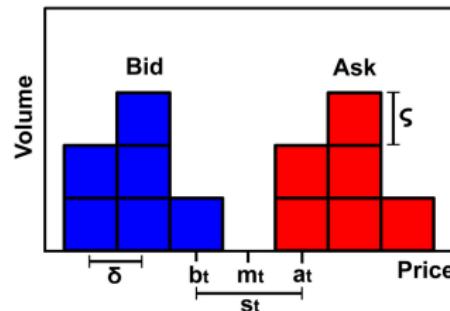
(a) Seismic imaging



(b) Brain fMRI



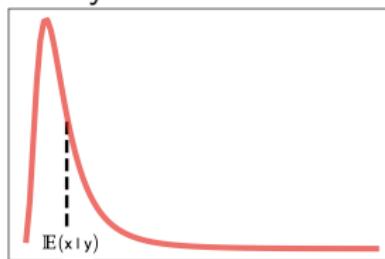
(c) Earth observation



(d) LOB analysis

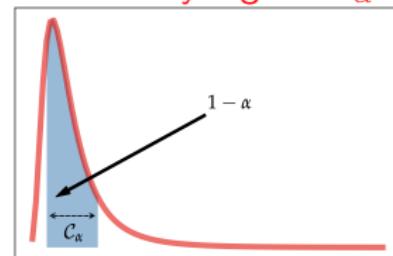
# Bayesian inference : Uncertainty quantification

Bayesian estimators



$$\arg \min \int h(\mathbf{x}) p(\mathbf{x} \mid \mathbf{y}) d\mathbf{x}$$

Credibility regions  $\mathcal{C}_\alpha$



$$\int_{\mathcal{C}_\alpha} p(\mathbf{x} \mid \mathbf{y}) d\mathbf{x} = 1 - \alpha, \quad \alpha \in (0, 1)$$

→ Computing such integrals is not straightforward

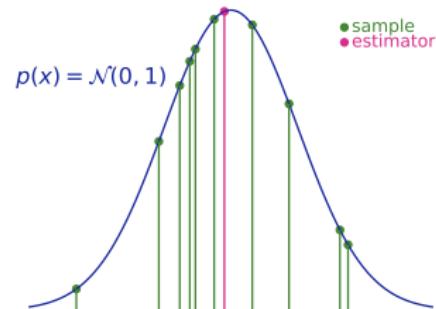
# Monte Carlo integration

One alternative lies in making use of sampling to approximate integration

$$\int h(\mathbf{x}) p(\mathbf{x} \mid \mathbf{y}) d\mathbf{x} \approx \frac{1}{N} \sum_{n=1}^N h\left(\mathbf{x}^{(n)}\right), \quad \mathbf{x}^{(n)} \sim p(\mathbf{x} \mid \mathbf{y})$$

## Sampling challenges :

- high-dimensional:  $\mathbf{x} \in \mathbb{R}^d$  with  $d \gg 1$
- composite:  $-\log p(\mathbf{x} \mid \mathbf{y}) = \sum_{i=1}^b U_i(\mathbf{x})$
- complicated: non-smooth/conjugate ...



# Sampling: Model based vs Data driven

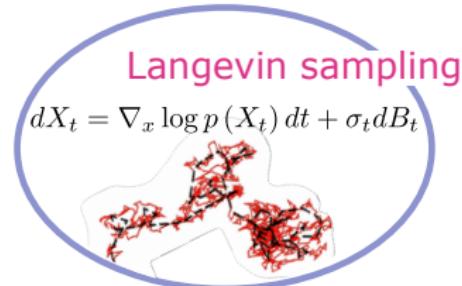
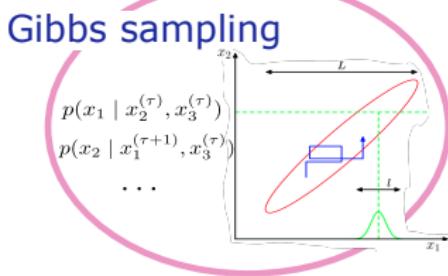
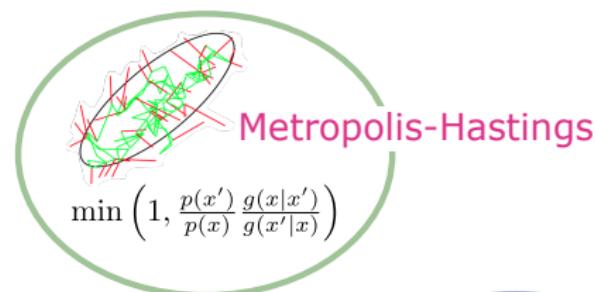
## Starting hypothesis

What information about  $p(\mathbf{x})$  is available ?

- model based, unnormalized density  $p(\mathbf{x}) \propto \exp[-U(\mathbf{x})]$
- data driven, samples  $\{\mathbf{x}_i\}_{i=0}^N \sim p(\mathbf{x})$

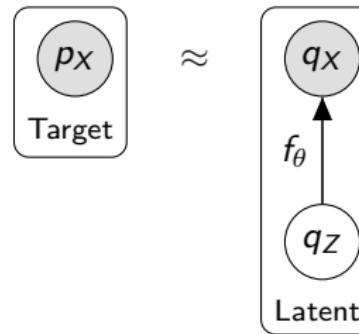
Field	Model based	Data driven
Information	$p(\mathbf{x}) \propto \exp[-U(\mathbf{x})]$	$\{\mathbf{x}_i\}_{i=0}^N \sim p(\mathbf{x})$
Methods	Monte Carlo	Learn mapping $f_{\sharp}q_Z \approx p_X$

# A myriad of Monte Carlo methods



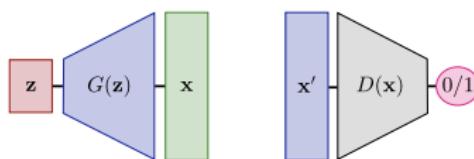
# What is deep generative modeling ?

- **Aim:** Approximate distribution  $q_X \approx p_X$  such that  $q_X := f_{\theta} \# q_Z$
- **A general approach :**
  - Samples  $\{x_i\}_{i=0}^N$  from  $p_X$  defined over  $\mathcal{X}$ .
  - Choose a simple **latent distribution**  $q_Z$  defined over  $\mathcal{Z}$ .
  - Learn a mapping  $f_{\theta} : \mathcal{Z} \rightarrow \mathcal{X}$  by minimizing  $D_{\text{Stat}}(p_X, f_{\theta} \# q_Z)$  over  $\theta$ .
- **Ancestral sampling :** Latent  $\mathbf{z} \sim q_Z \Rightarrow$  Target  $q_X \sim \hat{\mathbf{x}} = f(\mathbf{z})$

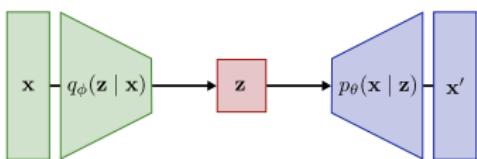


# A myriad of models

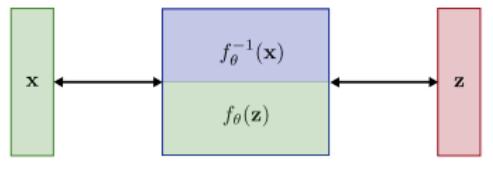
**GAN : Adversarial training**



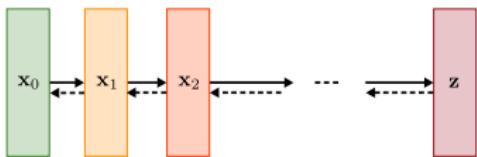
**VAE : ELBO**



**Normalizing Flow : KL**



**Diffusion models : Score matching**



# Contributions

## Submitted journal articles

- ▣ Coeurdoux et al. "Normalizing flow sampling with Langevin dynamics in the latent space", 2nd round JMLR
- ▣ Coeurdoux et al. "Plug-and-Play split Gibbs sampler: embedding deep generative priors in Bayesian inference", IEEE Transactions on Image Processing

## International conferences

- ▣ Coeurdoux et al. "Sliced-Wasserstein normalizing flows: beyond maximum likelihood training". ESANN 2022
- ▣ Coeurdoux et al. "Learning Optimal Transport Between two Empirical Distributions with Normalizing Flows". ECLM-PKDD 2022

## National conferences

- ▣ Coeurdoux et al. "Méthode MCMC plug-and-play avec a priori génératif profond". GRETSI 2023
- ▣ Coeurdoux et al. "Approximation du transport optimal entre distributions empiriques par flux de normalisation". GRETSI 2022

## Talk

- ♫ Workshop: Geostat Days, "Solving Inverse Problem with deep learning", Mines Paris PSL, Sept 2023
- ♫ Seminar: SIOP seminar, "Split Gibbs Plug-and-Play Sampler: Diffusion Models for inverse problem", University of Bordeaux, May 2023.
- ♫ Workshop: Interfacing Bayesian statistics and machine learning, "Langevin based Normalizing flow sampling", Bayes Centre, Edinburgh, Jan 2023
- ♫ Seminar: D2 Reading Group, "Normalizing flow sampling with Langevin dynamics in the latent space", Oxford University, Dec 2022
- ...

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# Plug-and-Play split Gibbs sampler: Motivation

## Inverse Problem

$$\begin{array}{ccc} \mathbf{y} & \approx & \mathcal{A}(\mathbf{x}) \\ \text{Observation} & & \text{Data acquisition} \end{array}$$

- **solve complex** ill-posed ML or inverse problems
- **big** data in high dimensions
- **good** performance
- **fast** inference algorithms
- **credibility intervals**

# The usual toolbox of inference

## ■ Optimization:

- problem  $\Rightarrow$  loss function
- efficient algorithms
- theoretical guarantees
- interpretability / functional analysis

## ■ Bayesian approaches:

- probabilistic models
- uncertainty quantification

## ■ Machine learning (deep):

- adaptive  $\Rightarrow$  relevant
- outstanding performance

Toward the best of all worlds?

# The optimization-based approach

Inverse problem  $\Rightarrow$  **cost function**

$$\mathbf{y} \cong \mathcal{A}(\mathbf{x}) \quad \Rightarrow \quad \hat{\mathbf{x}} = \arg \min_{\mathbf{x}} f(\mathbf{x}, \mathbf{y}) + g(\mathbf{x})$$

⚠ Explicit regularizations are significantly outperformed by DNN

- Half quadratic splitting (HQS)

$$L_\rho^{(\text{HQS})}(\mathbf{x}, \mathbf{z}) = f(\mathbf{x}, \mathbf{y}) + g(\mathbf{z}) + \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2,$$

- Decomposes into simpler sub problems:

$$\mathbf{x} \leftarrow \text{prox}_f(\mathbf{z}) = \arg \min_{\{\mathbf{x}\}} L_\rho^{(\text{HQS})}(\mathbf{x}, \mathbf{z}) = \arg \min_{\{\mathbf{x}\}} f(\mathbf{x}, \mathbf{y}) + \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2$$

$$\mathbf{z} \leftarrow \text{prox}_g(\mathbf{x}) = \arg \min_{\{\mathbf{z}\}} L_\rho^{(\text{HQS})}(\mathbf{x}, \mathbf{z}) = \arg \min_{\{\mathbf{z}\}} g(\mathbf{z}) + \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2$$

- **Plug-and-Play (PnP)  $\Leftarrow$  uses pretrained DL denoisers**

# The augmented Bayesian approach

Asymptotically exact data augmentation :

$$p(\mathbf{x} | \mathbf{y}) \propto \exp [-f(\mathbf{x}, \mathbf{y}) - g(\mathbf{x})]$$



$$p(\mathbf{x}, \mathbf{z} | \mathbf{y}) \propto \exp [-f(\mathbf{x}, \mathbf{y}) - g(\mathbf{z})] \text{ knowing that } \mathbf{x} = \mathbf{z}$$

## Proposed approach

systematic & simple way to relax  $p(\mathbf{x}, \mathbf{z} | \mathbf{y})$  leading to efficient algorithms

$$\int p_\rho(\mathbf{x}, \mathbf{z} | \mathbf{y}) d\mathbf{z} \xrightarrow[\rho \rightarrow 0]{} p(\mathbf{x} | \mathbf{y})$$

→ How to build  $p_\rho(\mathbf{x}, \mathbf{z} | \mathbf{y})$  ?

# On building $p_\rho$

A natural manner to construct  $p_\rho$  is to define:

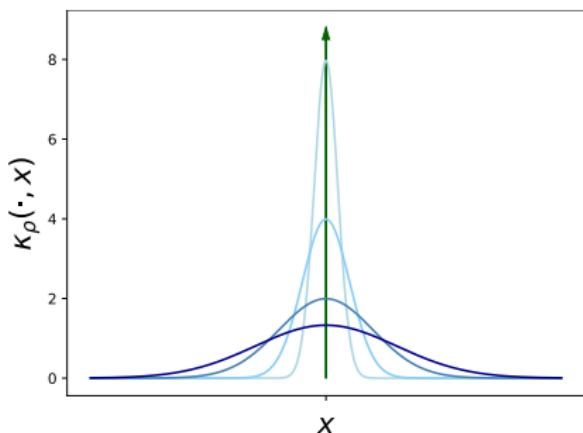
$$p_\rho(\mathbf{x}, \mathbf{z} \mid \mathbf{y}) \propto \exp [-f(\mathbf{x}, \mathbf{y}) - g(\mathbf{z})] \kappa_\rho(\mathbf{z}, \mathbf{x})$$

Where :

$$\kappa_\rho(\cdot, \mathbf{x}) \xrightarrow[\rho \rightarrow 0]{\text{weak}} \delta_{\mathbf{x}}(\cdot)$$

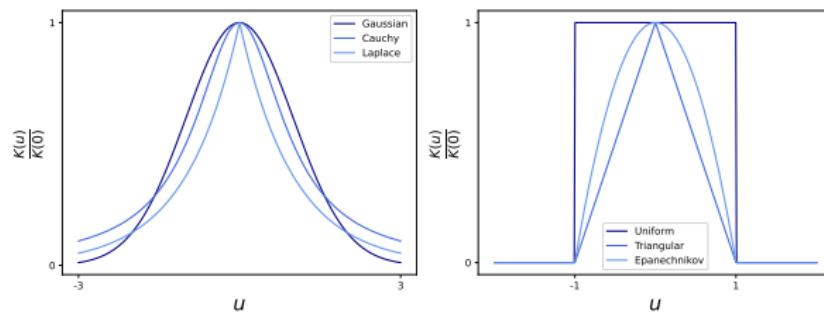
such that :

$$\|p - p_\rho\|_{\text{TV}} \xrightarrow[\rho \rightarrow 0]{} 0$$



$$\text{Kernel choice } \kappa_\rho(\mathbf{z}, \boldsymbol{\theta}) \propto \rho^{-d} K\left(\frac{\mathbf{z}-\boldsymbol{\theta}}{\rho}\right)$$

name	support	$K(u)$
Gaussian	$\mathbb{R}$	$\frac{1}{\sqrt{2\pi}} \exp(-u^2/2)$
Cauchy	$\mathbb{R}$	$\frac{1}{\pi(1+u^2)}$
Laplace	$\mathbb{R}$	$\frac{1}{2} \exp(- u )$
Dirichlet	$\mathbb{R}$	$\frac{\sin^2(u)}{\pi u^2}$
Uniform	$[-1, 1]$	$\frac{1}{2} \mathbb{I}_{ u \leq 1}$
Triangular	$[-1, 1]$	$(1 -  u ) \mathbb{I}_{ u \leq 1}$
Epanechnikov	$[-1, 1]$	$\frac{3}{4} (1 - u^2) \mathbb{I}_{ u \leq 1}$



→ Similarity with "noisy" ABC methods (Marin et al. 2012; Wilkinson 2013)

# Bias associated with Gaussian smoothing

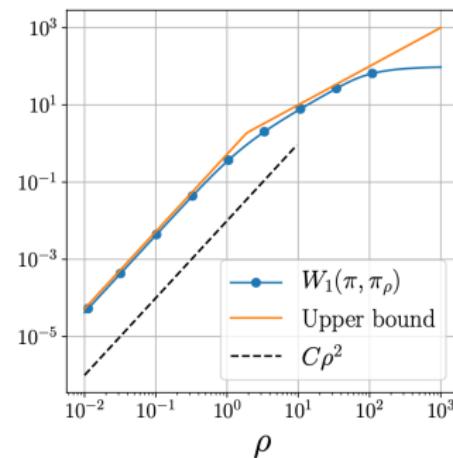
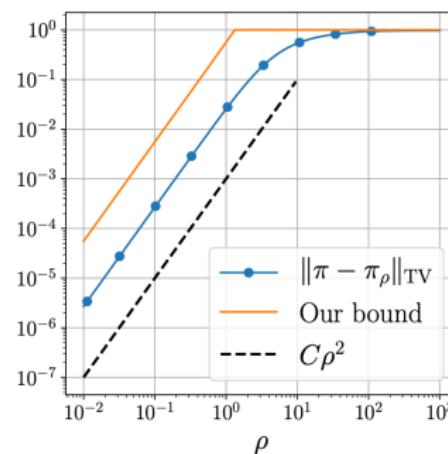
$$p_{\rho}(\mathbf{x} \mid \mathbf{y}) \propto \int_{\mathbb{R}^d} \exp \left[ \underbrace{-f(\mathbf{x}, \mathbf{y}) - g(\mathbf{z})}_{U(x)} - \underbrace{\frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2}_{\log \kappa_\rho} \right] d\mathbf{z}$$

Distance	Upper bound	Main assumptions on $U(\cdot)$
	$\rho 2\sqrt{d}L + o(\rho)$	$L$ -Lipschitz
$\ p_{\rho} - p\ _{\text{TV}}$	$\frac{1}{2}\rho^2 Md$	$M$ -smooth
	$\frac{1}{2}\rho^2 Md + o(\rho^2)$	$M$ -smooth & strongly convex
$W_1(p_{\rho}, p)$	$\min \left( \rho\sqrt{d}, \frac{1}{2}\rho^2\sqrt{Md} \right)$	$M$ -smooth & strongly convex

# Bias associated with Gaussian smoothing

Illustration of these bounds for an univariate Gaussian toy example :

$$p(\mathbf{x}) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{\mathbf{x}^2}{2\sigma^2}} \quad p_\rho(\mathbf{x}) = \frac{1}{\sqrt{2\pi(\sigma^2 + \rho^2)}} e^{-\frac{\mathbf{x}^2}{2(\sigma^2 + \rho^2)}}$$



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# Splitted Gibbs sampling: conditional distributions

**Goal sample from posterior:**

$$p(\mathbf{x}) \propto \exp [-f(\mathbf{x}, \mathbf{y}) - g(\mathbf{x})]$$

↓ Approx

$$p_{\rho}(\mathbf{x}, \mathbf{z}) \propto \exp \left[ -f(\mathbf{x}, \mathbf{y}) - g(\mathbf{z}) - \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2 \right]$$

Full conditional distributions under the split distribution  $p_{\rho}$  :

$$p(\mathbf{x} | \mathbf{z}, \mathbf{y}; \rho^2) \propto \exp \left[ -f(\mathbf{x}, \mathbf{y}) - \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2 \right] \quad (1)$$

$$p(\mathbf{z} | \mathbf{x}; \rho^2) \propto \exp \left[ -g(\mathbf{z}) - \frac{1}{2\rho^2} \|\mathbf{z} - \mathbf{x}\|_2^2 \right] \quad (2)$$

**Note that  $f$  and  $g$  are now separated in 2 distinct distributions<sup>2</sup>.**

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<sup>2</sup>Gibbs sampling: *Robert and Cassela, Springer 1999*

# Splitted Gibbs sampling: conditional distributions

**First Gibbs kernel** → task dependent  $f(\mathbf{x}, \mathbf{y})$ :

$$p(\mathbf{x} | \mathbf{z}, \mathbf{y}; \rho^2) \propto \exp \left[ -f(\mathbf{x}, \mathbf{y}) - \frac{1}{2\rho^2} \|\mathbf{x} - \mathbf{z}\|_2^2 \right]$$

Can be sampled using state of the art methods:

- **Gaussian forward model**: Fourier or Aux-V1 or E-PO<sup>3</sup>
- **Other forward model**: P-MYULA<sup>4</sup>= proximal MCMC<sup>5</sup>

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<sup>3</sup>Hight dim Gaussian sampling: *Vono et al., SIAM Review, 2022*

<sup>4</sup>P-MYULA: *Durmus et al., SIAM IS, 2018*

<sup>5</sup>Proximal MCMC: *M. Pereyra, Stat Comput, 2016*

# Splitted Gibbs sampling: conditional distributions

**Second Gibbs kernel** → prior dependent  $g(\textcolor{violet}{z})$ :

$$p(\textcolor{violet}{z} \mid \textcolor{violet}{x}; \rho^2) \propto \exp \left[ -g(\textcolor{violet}{z}) - \frac{1}{2\rho^2} \|\textcolor{violet}{z} - \textcolor{violet}{x}\|_2^2 \right]$$

Posterior of a Gaussian corruption of  $\textcolor{violet}{x}$  with prior  $g(\textcolor{violet}{z})$

- **Generative models:** DVAE, DGAN, DDPM<sup>6</sup>

## Proposed approach

Replace inefficient explicit prior by a deep generative denoiser → DDPM.

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<sup>6</sup>DDPM: Ho et al., NeurIPS, 2020

# Denoising Diffusion Probabilistic Models<sup>7</sup>

- Forward diffusion:  $p(x_t | x_{t-1}) = \mathcal{N}(x_t; \sqrt{1 - \beta(t)}x_{t-1}, \beta(t)\mathbf{I})$
- Reverse denoising:  $q_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

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<sup>7</sup>Visual: *Song and Ermon, NeurIPS, 2019*

# DDPM as stochastic denoisers

The denoising step of SGS is done as follows:

- 1 Infer the std of the noisy input using an estimator  $\hat{\sigma} = \Phi(\textcolor{red}{x})$
- 2 Deduce the starting time  $\hat{t}^* = \alpha^{-1}(\hat{\sigma}^2)$
- 3 Start the backward diffusion at  $\hat{t}^*$  and denoise using  $q_\theta(\textcolor{red}{x}_{t-1} \mid \textcolor{red}{x}_t)$

Note that

- a noise level  $\alpha(t^*)$  is associated to a unique instant  $t^*$
- $t^*$  adjusts the amount of imposed regularization

# DDPM as stochastic denoisers

Transition from the noise-free image  $x_0$  to noisy image  $x_t$ :

$$p(x_t | x_0) = \mathcal{N}(x_t; \sqrt{\bar{\alpha}(t)}x_0, \alpha(t)\mathbf{I})$$

where  $\alpha(t) = \prod_{j=1}^t (1 - \beta(j))$  and  $\bar{\alpha}(t) = 1 - \alpha(t)$

Any image  $x_t$  is a noisy version of  $x_0$  corrupted by a Gaussian noise of covariance  $\alpha(t)\mathbf{I}$ .

# Algorithm

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**Algorithm 1:** PnP-SGS using DDPM
 

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**Input :** Parameter  $\rho^2$ , total number of iterations  $N_{\text{MC}}$ , number of burn-in iterations  $N_{\text{bi}}$ , pre-trained DDPM  $s_\theta(\cdot, \cdot)$ , scheduling variance function  $\alpha(\cdot)$ , initialization  $\mathbf{z}^{(0)}$

```

1 for  $n \leftarrow 1$  to  $N_{\text{MC}}$  do
2   # Sampling the variable of interest  $\mathbf{x}^{(n)}$ 
3   Draw  $\mathbf{x}^{(n)} \sim p(\mathbf{x} \mid \mathbf{z}, \mathbf{y}; \rho^2)$  according to (6)
4   # Estimating noise level in  $\mathbf{x}^{(n)}$ 
5   Set  $\hat{\sigma} = \Phi(\mathbf{x}^{(n)})$  using [38]
6   # Setting the number of diffusion steps to denoise  $\mathbf{x}^{(n)}$ 
7   Set  $\hat{t}^* = \alpha^{-1}(\hat{\sigma}^2)$ 
8   # Sampling the splitting variable  $\mathbf{z}^{(n)}$  according to (7)
9   Set  $\mathbf{u}_{\hat{t}^*} = \mathbf{x}^{(n)}$ 
10  for  $j \leftarrow \hat{t}^*$  downto 1 do
11    | Draw  $\mathbf{u}_{j-1} \sim q_\theta(\mathbf{u}_{j-1} \mid \mathbf{u}_j)$  according to (10)
12  end for
13  Set  $\mathbf{z}^{(n)} = \mathbf{u}_0$ 
14 end for

```

**Output:** Collection of samples  $\{\mathbf{x}^{(n)}, \mathbf{z}^{(n)}\}_{t=N_{\text{bi}+1}}^{N_{\text{MC}}}$  asymptotically distributed according to (4).

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# Mixing time

How many SGS iterations should I run to obtain a sample from  $p(\mathbf{x} \mid \mathbf{y})$ ?

This question can be answered by giving an upper bound on the so-called  $\epsilon$ -mixing time:

$$t_{\text{mix}}(\epsilon; \nu) = \min \left\{ t \geq 0 \mid D \left( \nu P_{\text{SGS}}^t, p \right) \leq \epsilon \right\}$$

where  $\epsilon > 0$ ,  $\nu$  is an initial distribution,  $P_{\text{SGS}}$  is the Markov kernel of SGS and  $D$  is a statistical distance.

→ We are here interested in providing explicit bounds w.r.t.  $d, \epsilon$  and regularity constants associated to  $U$ <sup>8</sup>.

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<sup>8</sup>Vono et al., JMLR

# Explicit convergence rates

## Assumptions

$U$  is  $M$ -smooth &  $m$ -strongly convex, starting from  $\nu = \mathcal{N}(\mathbf{x}^*, M^{-1}\mathbf{I}_d)$

- $\forall \epsilon \in (0, 1)$ , with  $\rho^2 \leq \frac{\epsilon}{dM}$
- for  $t \geq t_{\text{mix}}(\epsilon; \nu)$  where :

$$t_{\text{mix}}(\epsilon; \nu) = \frac{\log\left(\frac{2}{\epsilon}\right) + C/2}{K_{\text{SGS}}}$$

Where :

$$K_{\text{SGS}} = \frac{m\rho^2}{1+m\rho^2} \quad \text{and} \quad C = \frac{5d}{8} + \frac{d}{2} \log\left(\frac{M}{m}\right)$$

- We have :

$$\|\nu P_{\text{SGS}}^t - p\|_{\text{TV}} \leq \epsilon$$

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# Image Inpainting

We consider the following linear model

$$\mathbf{y} = \mathbf{H}\mathbf{x} + \mathbf{n}$$

the likelihood function associated with the observation  $\mathbf{y}$  writes

$$p(\mathbf{y} | \mathbf{x}) \propto \exp \left[ -\frac{1}{2} (\mathbf{H}\mathbf{x} - \mathbf{y})^T \boldsymbol{\Omega} (\mathbf{H}\mathbf{x} - \mathbf{y}) \right].$$

Where  $\mathbf{H} \in \{0, 1\}^{N \times M}$  is a binary matrix associated and  $\boldsymbol{\Omega}^{-1} = \sigma^2 \mathbf{I}_M$ .

# Image Inpainting

the proposed PnP-SGS algorithm yields the conditional distribution defined here as

$$p(\mathbf{x} \mid \mathbf{z}, \mathbf{y}; \rho^2) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{\mathbf{x}}, \mathbf{Q}_{\mathbf{x}}^{-1})$$

with

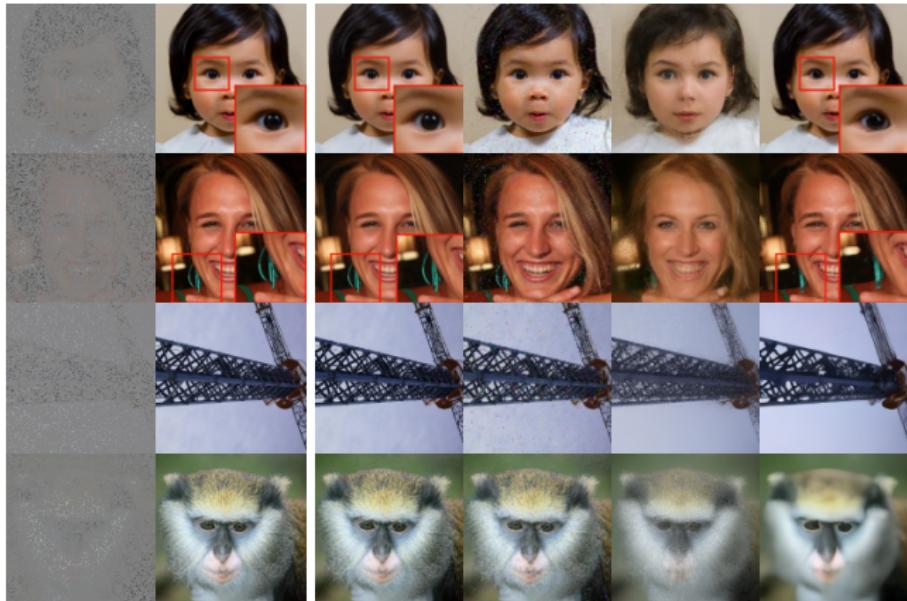
$$\begin{cases} \mathbf{Q}_{\mathbf{x}} = \frac{1}{\sigma^2} \mathbf{H}^T \mathbf{H} + \frac{1}{\rho^2} \mathbf{I}_N \\ \boldsymbol{\mu}_{\mathbf{x}} = \mathbf{Q}_{\mathbf{x}}^{-1} \left( \frac{1}{\sigma^2} \mathbf{H}^T \mathbf{y} + \frac{1}{\rho^2} \mathbf{z} \right). \end{cases}$$

From the Sherman-Morrison-Woodbury formula, we have:

$$\mathbf{Q}_{\mathbf{x}}^{-1} = \rho^2 \left( \mathbf{I}_N - \frac{\rho^2}{\sigma^2 + \rho^2} \mathbf{H}^T \mathbf{H} \right).$$

Which can be conducted efficiently with the exact perturbation-optimization (E-PO) algorithm.

# Image inpainting



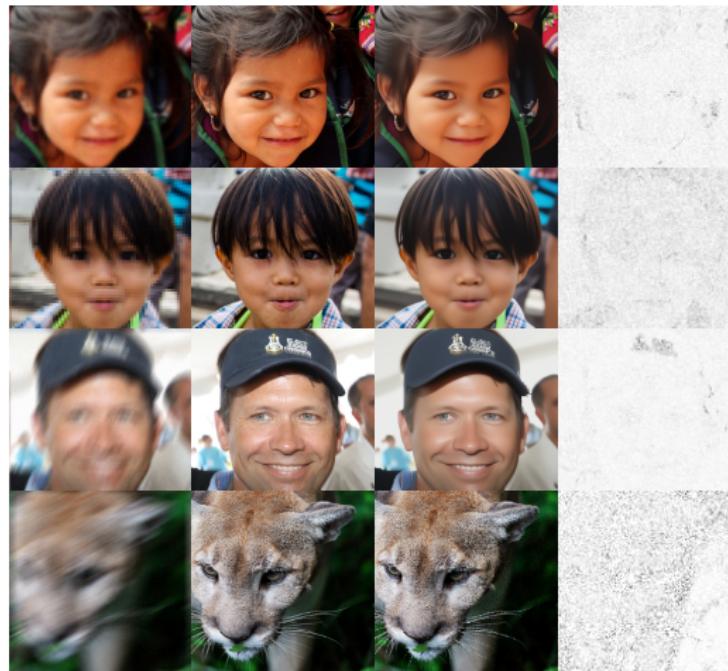
From left to right: measure, true, PnP-SGS, TV-SGS, DDRM, MCG.

# Image inpainting



From left to right: measure, true, PnP-SGS (MMSE)

# MMSE estimation



From top to bottom: Gaussian blur, motion blur, superresolution.

# MMSE estimation



# Quantitative evaluation

	FID ↓	LPIPS ↓	PSNR ↑	SSIM ↑
PnP-SGS	<b>38.36</b>	<b>0.144</b>	<b>23.59</b>	<b>0.813</b>
TV-SGS	71.12	0.785	21.09	0.524
PnP-ADMM	123.61	0.692	<u>22.41</u>	0.325
TV-ADMM	181.56	0.463	22.03	<u>0.784</u>
Score-SDE	76.54	0.612	13.52	0.437
DDRM	69.71	0.587	9.19	0.319
MCG	<u>39.26</u>	<u>0.286</u>	21.57	0.751

Benchmark for FFHQ  $256 \times 256$  with 1000 images.

PnP-SGS	TV-SGS	PnP-ADMM	Score-SDE	DDRM	MCG
13.81	218.90	3.63	36.71	29.03	80.10

Inpainting: computational times (s.)

# Black Holes image reconstruction - VLBI interferometer

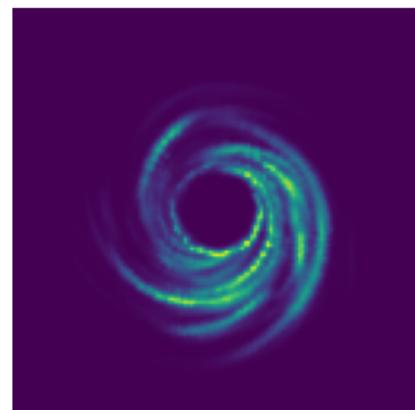
The Event Horizon Telescope measures complex-visibility  $V$  :

$$V(u, v) = \int I(x, y) e^{-2\pi i(ux+vy)} dx dy$$

Signal corrupted by the atmosphere,  
with the complex term  $g$  :

$$\tilde{V}_{ij} = g_i g_j^* V_{ij}$$

and Complex Gaussian thermal  
noise.



# Conclusion: PnP-SGS

- Plug-and-play split Gibbs sampler (PnP-SGS):
  - Bridge MCMC and Plug-and-Play methods
  - Explicit convergence rates and mixing times
  - Credibility intervals
  - Fast and scalable sampling
  - general: using any deep generative denoiser
  - State of the art: on image processing problems
- Perspectives:
  - Study theoretical denoising properties of deep generative models
  - Adaptive PnP-SGS : find a sequence  $\rho_k \in \mathcal{N}$

Thank you for your attention!  
Questions ?



Joint work with Nicolas Dobigeon, Pierre Chainais, Arnaud Doucet & Paul Tiede

# Appendix

# Poisson and non-Gaussian

Let consider the observation of some image  $\mathbf{y} \in \mathbb{N}^m$ , damaged and contaminated by Poisson noise

$$y_i \stackrel{\text{iid.}}{\sim} \mathcal{P}([\mathbf{Hx} + \mathbf{b}]_i)$$

the likelihood distribution is rewritten as follows

$$p(\mathbf{y} | \mathbf{x}) \propto \exp(-f_1(\mathbf{Hx}; \mathbf{y}))$$

where

$$f_1(\mathbf{Hx}; \mathbf{y}) = \sum_{i=1}^m -y_i \log ([\mathbf{Hx} + \mathbf{b}]_i) + [\mathbf{Hx} + \mathbf{b}]_i$$

By the application of Bayes' rule, the AXDA envelope of the posterior distribution writes

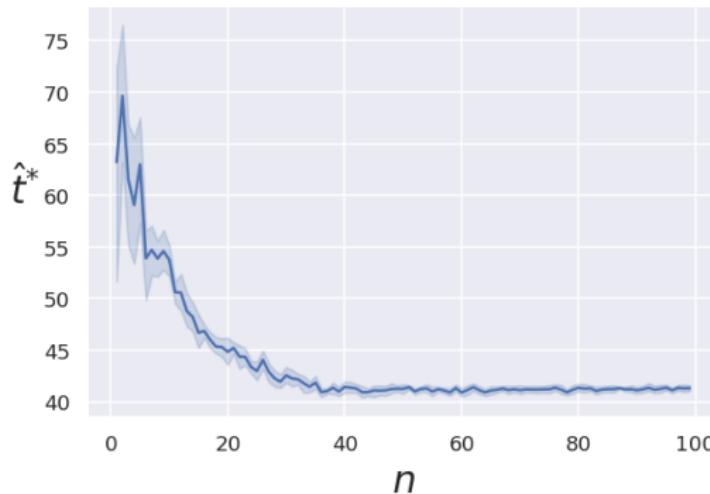
$$\pi_\rho(\mathbf{x}, \mathbf{z}) \propto \exp \left( -f_1(\mathbf{Hx}) - g(\mathbf{z}) + \frac{1}{2\rho} \|\mathbf{x} - \mathbf{z}\|_2^2 \right)$$

# Comparison with ULA

<b>Distance</b>	<b>Upper Bound</b>	<b>Main assumptions</b>
$\ \pi_\rho - \pi\ _{\text{tv}}$	$\frac{1}{2}\rho^2 M_1 d$	$M$ -smooth
$\ \pi_{\text{ULA}} - \pi\ _{\text{tv}}$	$\sqrt{2Md} \cdot \rho$	$M$ -smooth & convex
$W_1(\pi_\rho, \pi)$	$\min\left(\rho\sqrt{d}, \frac{1}{2}\rho^2\sqrt{Md}\right)$	$M$ -smooth, $m$ -strongly convex
$W_1(\pi_{\text{ULA}}, \pi)$	$\sqrt{2\frac{M}{m}d} \cdot \rho$	$M$ -smooth, $m$ -strongly convex

→ Higher order approximation based on the explicit form of  $\pi_\rho$ .

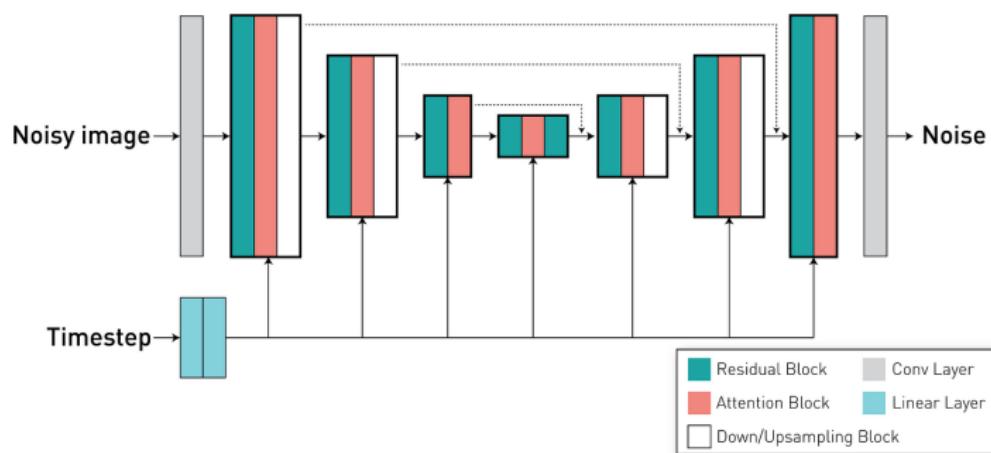
# Evolution of $\hat{t}$



**Figure:** Inpainting: evolution of  $\hat{t}^*$  along the PnP-SGS iterations ( $T = 1000$ ). Results have been averaged over 100 runs conducted on the same image. Shaded areas stand for the corresponding standard deviation.

# Diffusion model implementation considerations

Diffusion models often use U-Net architectures with ResNet blocks and self-attention



Time representation: sinusoidal positional embeddings or random Fourier features.