

Monte Carlo sampling and deep generative models for Bayesian inference

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November 23th, 2023

Bayesian inference

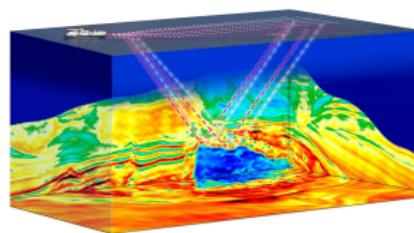
x: unknown object of interest
y: available data (observation)

Update of prior information with available data¹:

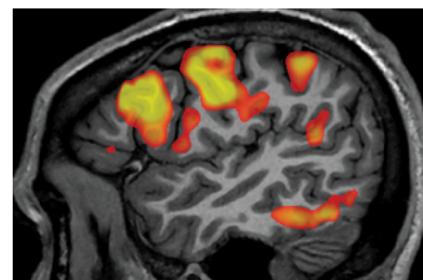
$$\begin{array}{ccc}
 \text{Prior} & \times & \text{Likelihood} \rightarrow \text{Posterior} \\
 p(x) & & p(y | x) \quad p(x | y) \\
 \uparrow & & \uparrow \\
 \text{pre-observation} & & \text{acquisition} \\
 \text{knowledge} & & \text{process} \\
 \uparrow & & \uparrow \\
 \text{best} & & \text{guess}
 \end{array}$$

¹For complete review, see *Robert and Casella, 1999*

Various applications



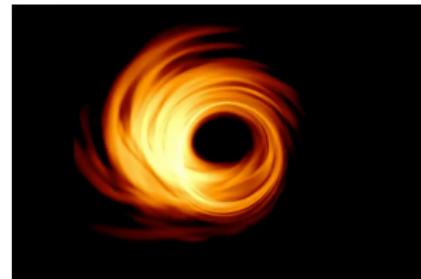
(a) Seismic imaging



(b) Brain fMRI



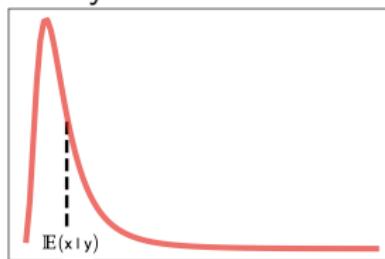
(c) Earth observation



(d) Astrophysics

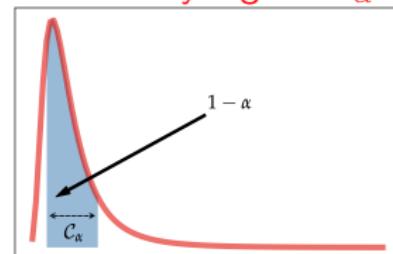
Bayesian inference : Uncertainty quantification

Bayesian estimators



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

Credibility regions \mathcal{C}_α



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

→ Computing such integrals is not straightforward

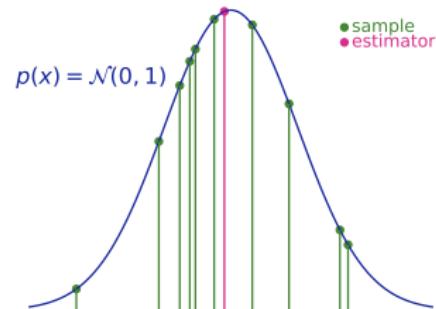
Monte Carlo integration

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

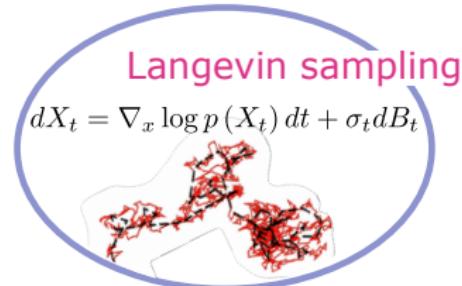
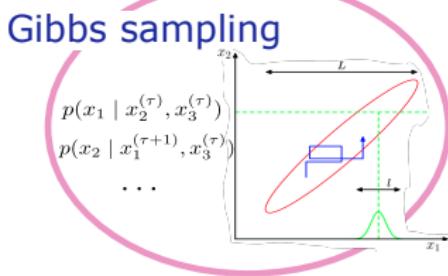
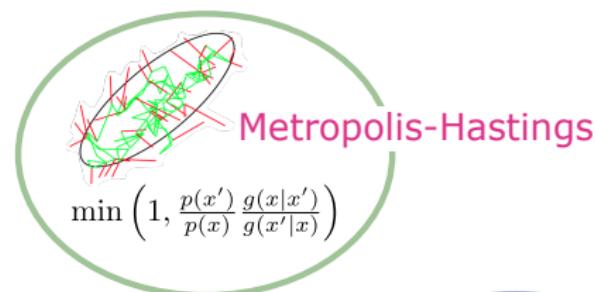
Starting hypothesis

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

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

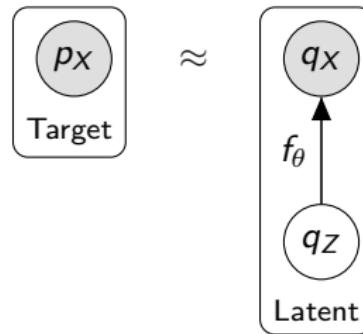
| Field | Model based | Data driven |
|-------------|----------------------------------------------|-----------------------------------------------|
| Information | $p(\mathbf{x}) \propto \exp[-U(\mathbf{x})]$ | $\{\mathbf{x}_i\}_{i=0}^N \sim p(\mathbf{x})$ |
| Methods | Monte Carlo | Learn mapping $f_{\sharp}q_Z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

A myriad of Monte Carlo methods



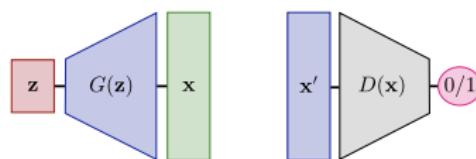
What is deep generative modeling ?

- **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 θ .
- **Ancestral sampling :** Latent $\mathbf{z} \sim q_Z \Rightarrow$ Target $q_X \sim \hat{\mathbf{x}} = f(\mathbf{z})$

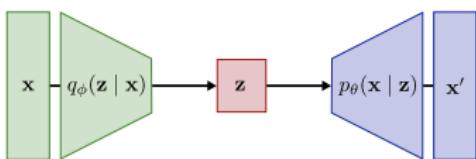


A myriad of models

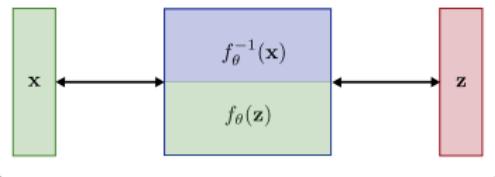
GAN : Adversarial training



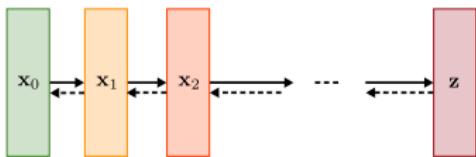
VAE : ELBO



Normalizing Flow : KL



Diffusion models : Score matching

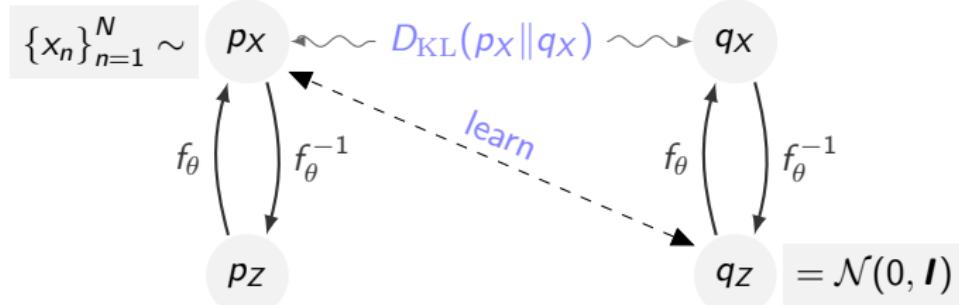


- 1 Introduction and context
- 2 Normalizing Flow SAmpling In Latent Space (NF-SAILS)
 - Motivations
 - Implications of topological mismatch
 - Sampling in the latent space
 - Experiments
- 3 Plug-and-Play split Gibbs sampler (PnP-SGS)
 - Split-Gibbs Sampling
 - DDPM
 - PnP-SGS
 - Numerical Experiments
- 4 Conclusion

Normalizing flows

Architecture

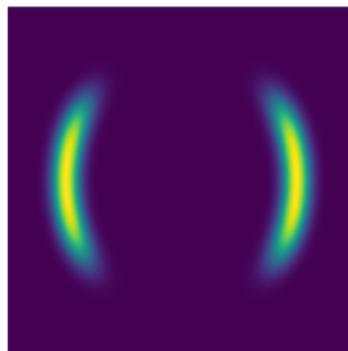
- **Bijective:** $f_\theta(\mathbf{z}) = \mathbf{x}$ and $f_\theta^{-1}(\mathbf{x}) = \mathbf{z}$
- **Aim:** $p_X \approx q_X := f_\# q_Z$
- **Types:** RealNVP, MAF, GLOW, NICE, FFJORD, ...
- **Change of variables formula:** $q_X(\mathbf{x}) = q_Z(f_\theta^{-1}(\mathbf{x})) \left| J_{f_\theta^{-1}}(\mathbf{x}) \right|$



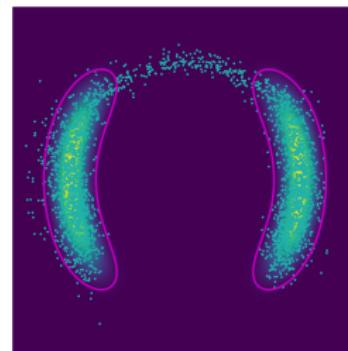
Problem statement

Pathological behaviors of flow based models:

- Incapacity to model multi-components distributions
- Prescribes high likelihood to OOD data.



p_x



q_x

Topological mismatch

- The mapping f is continuous, bijective and differentiable.
- q_X and q_Z are homeomorphic \rightarrow maintain topological properties.
- Then the push-forward operator f_{\sharp} can yield $q_X = p_X$ only if

$$\text{supp}(p_X) = \overline{f(\text{supp}(q_Z))}$$

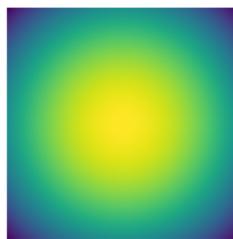
where \bar{B} is the closure of set B .

Proposition

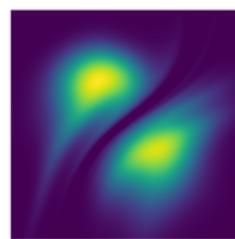
Let q_Z and p_X denote distributions defined on \mathbb{R}^d . Assume that $\text{supp}(q_Z) \neq \text{supp}(p_X)$. For any sequence of measurable, differentiable Lipschitz functions $f_t : \mathbb{R}^{d_Z} \rightarrow \mathbb{R}^{d_X}$, if $f_{t\sharp} q_Z \xrightarrow{\mathcal{D}} p_X$ when $t \rightarrow +\infty$, then

$$\lim_{t \rightarrow \infty} \sup_{z \in \mathcal{Z}} (\|J_{f_t}(z)\|) = +\infty$$

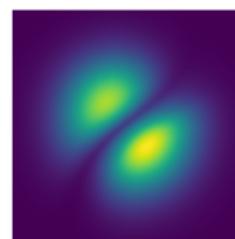
Topological mismatch



$$q_Z = \mathcal{N}(0, I)$$



$$p_Z := f_{\sharp}^{-1} p_X$$



$$\tilde{q}_Z(z) = q_Z(z) |J_f(z)|^{-1}$$

Implications :

- NF partitions the latent space in regions separated by exploding J_f .
- Zones with exploding J_f correspond to in between modes with low probability areas in p_X .

→ Sample by avoiding high J_f areas

Global kernel

NF models push any distribution toward $\mathcal{N}(0, I)$, making it a perfect proposal distribution in a Metropolis-Hastings. The corresponding acceptance ratio writes:

$$\begin{aligned}\alpha_{\text{I-MH}}(\mathbf{z}_k, \mathbf{z}') &= \min \left(1, \frac{\tilde{q}_Z(\mathbf{z}') q_Z(\mathbf{z}_k)}{\tilde{q}_Z(\mathbf{z}_k) q_Z(\mathbf{z}')} \right) \\ &= \min \left(1, \frac{|J_f(\mathbf{z}_k)|}{|J_f(\mathbf{z}')|} \right)\end{aligned}$$

Algorithm 4: Sampling kernel $\mathcal{K}_{\text{I-MH}}(\cdot)$.

Input: trained NF $f(\cdot)$, current state z_k of the sampler.

```

/* Draw candidate */  

1 Draw  $z' \sim \mathcal{N}(0, 1)$  /* Accept/reject procedure */  

2 Draw  $u \sim \mathcal{U}(0, 1)$   

3 if  $u < \alpha_{\text{I-MH}}(z_k, z')$  then  

4   | Set  $z_{k+1} = z'$   

5 else  

6   | Set  $z_{k+1} = z_k$   

Output: New state  $z_{k+1} = \mathcal{K}_{\text{I-MH}}(z_k)$  of the sampler.
```

Sampling in the latent space

The Unadjusted Langevin Algorithm (ULA) which targets q_X :

$$dX_t = \nabla_x \log q_X (X_t) dt + \sigma_t dB_t$$

Following Ito's lemma with second order truncation :

$$df^{-1}(X_t) = J_{f^{-1}}(X_t) \nabla_x \log q_X (X_t) dt + \sigma_t J_{f^{-1}}(X_t) dB_t$$

which can be rewritten as :

$$\begin{aligned} dZ_t &= J_f^{-1}(Z_t) J_f^{-1}(Z_t) \nabla_z \log \tilde{q}_Z (Z_t) dt + \sigma_t J_f^{-1}(Z_t) J_f^{-1}(Z_t) dB_t \\ &= \boxed{G^{-1}(Z_t) \nabla_z \log \tilde{q}_Z (Z_t) dt + \sigma_t \sqrt{G^{-1}(Z_t)} dB_t} \end{aligned}$$

With $G^{-1}(z) = [J_f^{-1}(z)]^2$ and $\tilde{q}_Z(z) = q_Z(z) |J_f(z)|^{-1}$.

→ We recover the Riemann Manifold ULA which targets \tilde{q}_Z .

Riemannian manifold adjusted Langevin algorithm

- Discretization: Euler–Maruyama :

$$\mathbf{z}' = \mathbf{z} + \frac{\epsilon^2}{2} \cdot \mathcal{G}^{-1}(\mathbf{z}) \nabla_{\mathbf{z}} \log \tilde{q}_{\mathbf{z}}(\mathbf{z}) + \epsilon \cdot \sqrt{\mathcal{G}^{-1}(\mathbf{z})} \xi, \quad \xi \sim \mathcal{N}(0, I)$$

- Correction: Metropolis-Hastings rejection step :

$$g(\mathbf{z}' | \mathbf{z}) \propto |\mathcal{J}_f(\mathbf{z})| \exp \left[-\frac{1}{2\epsilon^2} \left\| \mathcal{J}_f(\mathbf{z}) (\mathbf{z}' - \mathbf{z}) + \frac{\epsilon^2}{2} \mathcal{J}_f^{-1}(\mathbf{z}) \nabla_{\mathbf{z}} \log \tilde{q}_{\mathbf{z}}(\mathbf{z}) \right\|^2 \right]$$

The samples are accepted with probability

$$\alpha_{\text{RMMALA}}(\mathbf{z}_k, \mathbf{z}') = \min \left(1, \frac{\tilde{q}_{\mathbf{z}}(\mathbf{z}') g(\mathbf{z}_k | \mathbf{z}')}{\tilde{q}_{\mathbf{z}}(\mathbf{z}_k) g(\mathbf{z}' | \mathbf{z}_k)} \right).$$

Efficient implementation

■ Efficient diffusion:

- Proposal scheme requires sampling from $\mathcal{N}(0, \epsilon^2 G^{-1}(\cdot)) \rightarrow \text{slow}$
- Alternatively, we take advantage of the 1st order expansion:

$$f^{-1} \left(\underbrace{f(\mathbf{z}_k) + \epsilon \xi}_{\mathbf{x}_k + \epsilon \xi} \right) \simeq \underbrace{\mathbf{z}_k}_{f^{-1} \circ f(\mathbf{z}_k)} + \epsilon J_{f^{-1}} \left(\underbrace{f(\mathbf{z}_k)}_{\mathbf{x}_k} \right) \xi$$

→ much faster to leverage the learned mapping f

■ Efficient latent score computation

Latent score $\tilde{s}_Z(\mathbf{z}) = J_f^{-1}(\mathbf{z}) \nabla_{\mathbf{z}} \log \tilde{q}_Z(\mathbf{z})$ appears in proposal and diffusion.

- Jacobian computation $J_f^{-1}(\mathbf{z})$ is slow in high dimension.
- The latent score can be expressed in the latent domain:

$$\nabla_{\mathbf{x}} \log q_X(\mathbf{x}) = J_f^{-1}(\mathbf{z}) \cdot \nabla_{\mathbf{z}} \log \tilde{q}_Z(\mathbf{z}) \quad \text{s.t. } \mathbf{x} = f(\mathbf{z})$$

Local kernel → RMMALA

Putting all together we have the following RMMALA:

Algorithm 3: Sampling kernel $\mathcal{K}_{\text{RMMALA}}(\cdot)$.

Input: trained NF $f(\cdot)$, time step ϵ , current state z_k of the sampler.

/* Draw the candidate */

1 Draw $\xi \sim \mathcal{N}(0, 1)$

2 Set $z' = f^{-1}(f(z_k) + \epsilon \cdot \xi) + \frac{\epsilon^2}{2} J_f^{-1}(z_k) \tilde{s}_Z(z_k)$

/* Accept/reject procedure */

3 Draw $u \sim \mathcal{U}(0, 1)$

4 if $u < \alpha_{\text{RMMALA}}(z_k, z')$ then

5 | Set $z_{k+1} = z'$

6 else

7 | Set $z_{k+1} = z_k$

Output: New state $z_{k+1} = \mathcal{K}_{\text{RMMALA}}(z_k)$ of the sampler.

→ Only sample local region, get stuck in each modes

NF-SAILS

NF-SAILS combines the transition kernels $\mathcal{K}_{\text{RMMALA}}$ and $\mathcal{K}_{\text{I-MH}}$:

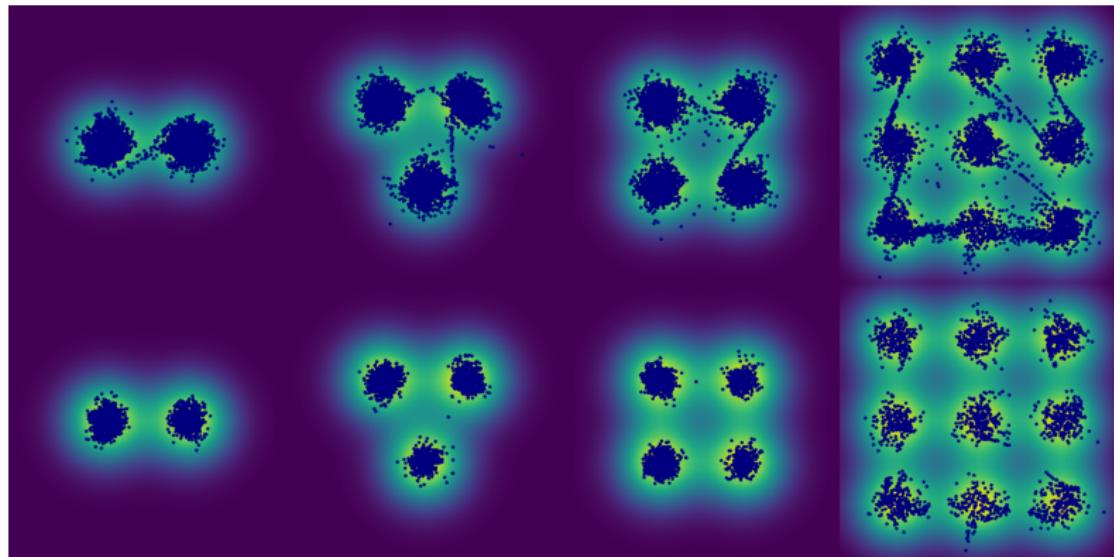
- Local search with probability p .
- Global search with probability $(1 - p)$.

Algorithm 5: NF-SAILS: NF SAmpling In the Latent Space.

```
Input: trained NF  $f(\cdot)$ , time step  $\epsilon$ , probability  $p$ 
/* Initialization */  
1 Draw  $z_0 \sim \pi_0(z)$   
2 for  $k = 0$  to  $K$  do
    /* Choose the kernel */  
    3 Draw  $u \sim \mathcal{U}(0, 1)$   
    4 if  $u < p$  then
        /* LOCAL EXPLORATION (see Algo. 3) */  
        5  $z_{k+1} = \mathcal{K}_{\text{RMMALA}}(z_k)$   
    else
        /* GLOBAL EXPLORATION (see Algo. 4) */  
        7  $z_{k+1} = \mathcal{K}_{\text{I-MH}}(z_k)$   
8 end
```

Output: Collection of samples $\{z_k\}_{k=1}^K$.

Multimodal toy examples



(top) Ancestral Sampling (Bottom) NF-SAILS

High dimensional experiments

| | ↓ bpd | ↓ FID |
|----------------|-------------|-------------|
| Naive sampling | 3.35 | 44.6 |
| NF-SAILS | 3.08 | 43.11 |
| WGAN-GP | N/A | 18.8 |



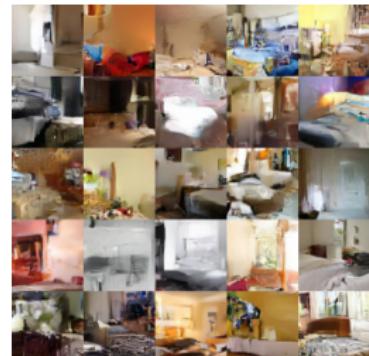
Cifar10

| | ↓ bpd | ↓ FID |
|----------------|-------------|--------------|
| Naive sampling | 1.03 | 15.82 |
| NF-SAILS | 0.96 | 14.12 |
| WGAN-GP | N/A | 12.89 |



CelebA

| | ↓ bpd | ↓ FID |
|----------------|-------------|-------------|
| Naive sampling | 2.38 | 8.91 |
| NF-SAILS | 2.11 | 7.86 |
| WGAN-GP | N/A | 9.56 |



LSUN (bedroom)

Conclusion: NF-SAILS

Problem

- Jacobian norm explodes for disjoint support distributions
- Existence of pathological areas in the latent space

Solutions

- Langevin sampling procedure over the latent space
- Riemanian manifold MALA
- Applied to any pre-trained NF

 Coeurdoux et al. "Normalizing flow sampling with Langevin dynamics in the latent space", Submitted to Machine Learning

 Workshop : Interfacing Bayesian statistics and machine learning, "Langevin based Normalizing flow sampling", Bayes Centre, Edinburgh, Jan 2023.

1 Introduction and context

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- Motivations
- Implications of topological mismatch
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3 Plug-and-Play split Gibbs sampler (PnP-SGS)

- Split-Gibbs Sampling
- DDPM
- PnP-SGS
- Numerical Experiments

4 Conclusion

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 Bayesian approach augmented by splitting

- Asymp. eXact Data Augmentation (AXDA)²:

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



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



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

- Asymptotic convergence in distribution:

$$\|\pi - \pi_p\|_{\text{TV}} \xrightarrow{\rho^2 \rightarrow 0} 0$$

²AXDA: Vono et al, *Journal of Computational and Graphical Statistics*, 2020

Splitted Gibbs sampling: conditional distributions

Full conditional distributions under the split distribution π_ρ :

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

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

Note that f and g are now separated in 2 distinct distributions³.

- Eq (1) can be sampled using state of the art methods:
 - **Gaussian variables:** Fourier or Aux-V1 or E-PO
 - **P-MYULA** = proximal MCMC
- Eq (2) is the Posterior of a Gaussian corruption of \mathbf{x} with prior $g(\mathbf{z})$
 - **Generative models:** DVAE, DGAN, DDPM

³SPA: Vono et al, IEEE Transactions on Signal Processing, 2019

Denoising Diffusion Probabilistic Models⁴

- 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: $q_\theta(x_{t-1} | x_t) = \mathcal{N}(x_{t-1}; \mu_\theta(x_t, t), \Sigma_\theta(x_t, t))$

⁴Visual: *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

Algorithm 1: PnP-SGS using DDPM

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

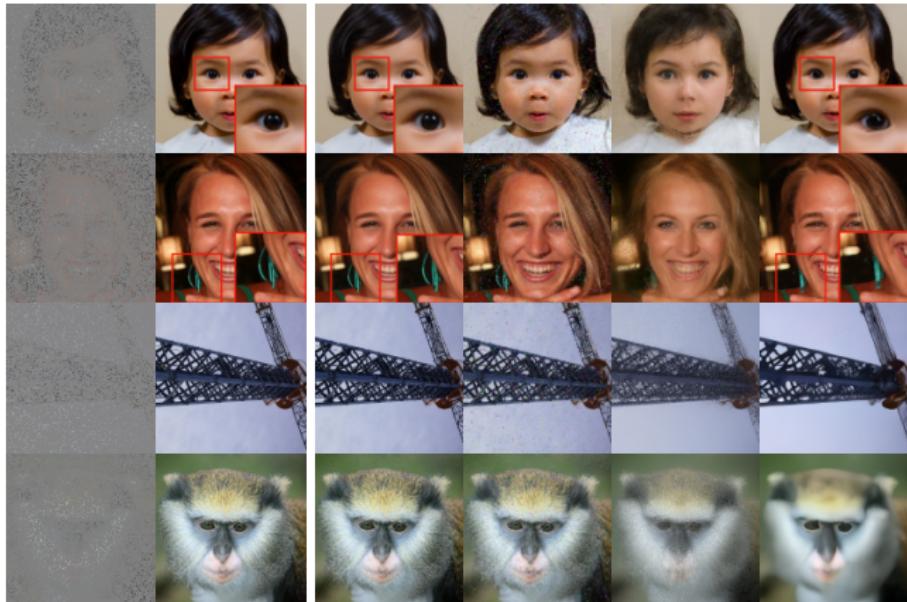
```

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

```

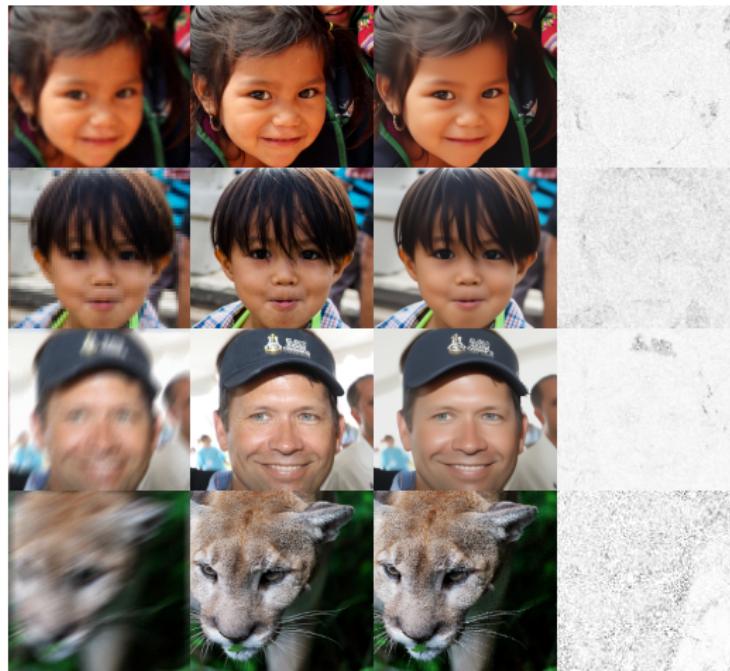
Output: Collection of samples $\{\mathbf{x}^{(n)}, \mathbf{z}^{(n)}\}_{t=N_{\text{bi}+1}}^{N_{\text{MC}}}$ asymptotically distributed according to (4).

Image inpainting



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

MMSE estimation



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

Quantitative evaluation

| | FID ↓ | LPIPS ↓ | PSNR ↑ | SSIM ↑ |
|-----------|--------------|--------------|--------------|--------------|
| PnP-SGS | 38.36 | 0.144 | 23.59 | 0.813 |
| 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 256×256 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.)

Conclusion: PnP-SGS

The plug-and-play split Gibbs sampler (PnP-SGS) provides:

- Bridge AXDA and Plug-and-Play methods
- Asymptotic convergence toward the posterior
- Credibility intervals
- Fast and scalable sampling
- General: using any deep generative denoiser.

→ No theoretical denoising properties of diffusion models yet

1 Introduction and context

2 Normalizing Flow SAmpling In Latent Space (NF-SAILS)

- Motivations
- Implications of topological mismatch
- Sampling in the latent space
- Experiments

3 Plug-and-Play split Gibbs sampler (PnP-SGS)

- Split-Gibbs Sampling
- DDPM
- PnP-SGS
- Numerical Experiments

4 Conclusion

Contributions

Submitted journal articles

-  Coeurdoux et al. "Normalizing flow sampling with Langevin dynamics in the latent space", Submitted to Machine Learning
-  Coeurdoux et al. "Plug-and-Play split Gibbs sampler: embedding deep generative priors in Bayesian inference", Submitted to 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
- ...