Plug-and-Play split Gibbs sampler: embedding deep generative priors in Bayesian inference

Pierre Chainais

N. Dobigeon, F. Cœurdoux (IRIT)

May 30, 2024

Collaborators

Nicolas Dobigeon, Florentin Cœurdoux, Maxime Vono

Image deblurring

Image deblurring

Image inpainting

Image inpainting

Confidence intervals

Motivations

$$
\mathbf{y} = \mathcal{A}(\mathbf{x}) + \mathbf{n}
$$

- \triangleright solve complex ill-posed ML or inverse problems
- \triangleright big data in high dimensions
- ▶ good performances
- \triangleright fast inference algorithms
- \blacktriangleright credibility intervals

with maybe some additional options such as:

- \blacktriangleright privacy preserving
- \blacktriangleright distributed computing

Bayesian approach + Monte Carlo method + machine learning?

Motivations

$$
\mathbf{y} = \mathcal{A}(\mathbf{x}) + \mathbf{n}
$$

- ▶ solve complex ill-posed ML or inverse problems
- \triangleright big data in high dimensions
- ▶ good performances
- \triangleright fast inference algorithms
- \blacktriangleright credibility intervals

with maybe some additional options such as:

- \blacktriangleright privacy preserving
- \blacktriangleright distributed computing

Bayesian approach $+$ Monte Carlo method + machine learning?

The usual toolbox of inference

▶ Optimization:

- problem \Rightarrow loss function
- **•** efficient algorithms
- theoretical guarantees
- \bullet interpretability / functional analysis

▶ Bayesian approaches:

- probabilitic models
- uncertainty quantification
- \blacktriangleright Machine learning (deep):
	- adaptive \Rightarrow relevant
	- outstanding performance

toward the best of all worlds?

PnP-SGS for inverse problems

State of the art performance $+$ credibility intervals

- y : available data = observations
- x: unknown object of interest

- y : available data = observations
- x: unknown object of interest

ˆx

- **y**: available data $=$ observations
- x: unknown object of interest

Credibility regions \mathcal{C}_{α}

$$
\int_{\mathcal{C}_{\alpha}} \pi(\mathbf{x}|\mathbf{y}) \mathrm{d}\mathbf{x} = 1 - \alpha
$$

- y : available data = observations
- x: unknown object of interest

Image to restore y

- y : available data = observations
- x: unknown object of interest

Restored image \hat{x}

- y : available data = observations
- x: unknown object of interest

Illustration: 2D Gaussian mixture model - MTM steps

Illustration: 2D Gaussian mixture model - MALA + MTM

Bayesian approach for imaging inverse problems

Linear Gaussian inverse problems

 $y = Ax + n$

 $A =$ damaging operator (blur, binary mask...) $\mathbf{n} \sim \mathcal{N}\left(\mathbf{0}_{d}, \sigma^{2} \mathbf{I}_{d}\right) = \text{noise}.$

Posterior distribution
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp \left[-\frac{1}{2\sigma^2} ||\mathbf{y} - \mathbf{A}\mathbf{x}||_2^2 - \lambda g(\mathbf{x})\right]
$$

where $g(x)$ = prior knowledge on solutions.

- **1** generally **high dimension** of the image, e.g. 1 million pixels,
- **2 generality** of the prior distribution of probability, cf. $g(x)$

Bayesian approach for imaging inverse problems Linear Gaussian inverse problems

 $y = Ax + n$

 $A =$ damaging operator (blur, binary mask...) $\mathbf{n} \sim \mathcal{N}\left(\mathbf{0}_{d}, \sigma^{2} \mathbf{I}_{d}\right) = \text{noise}.$

Posterior distribution
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp \left[-\frac{1}{2\sigma^2} ||\mathbf{y} - \mathbf{A}\mathbf{x}||_2^2 - \lambda g(\mathbf{x})\right]
$$

where $g(x) =$ prior knowledge on solutions.

- **1** generally **high dimension** of the image, e.g. 1 million pixels,
- **2 generality** of the prior distribution of probability, cf. $g(x)$

Bayesian approach for imaging inverse problems Linear Gaussian inverse problems

 $y = Ax + n$

 $A =$ damaging operator (blur, binary mask...) $\mathbf{n} \sim \mathcal{N}\left(\mathbf{0}_{d}, \sigma^{2} \mathbf{I}_{d}\right) = \text{noise}.$

Posterior distribution
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp \left[-\frac{1}{2\sigma^2} ||\mathbf{y} - \mathbf{A}\mathbf{x}||_2^2 - \lambda g(\mathbf{x})\right]
$$

where $g(x) =$ prior knowledge on solutions.

- \bullet generally **high dimension** of the image, e.g. 1 million pixels,
- **2 generality** of the prior distribution of probability, cf. $g(x)$

メロメ メタメ メミメ メミメ

Natural images as stochastic processes

Conjecture by D. Mumford & B. Gidas :

There exists simply described stochastic models for images :

- ¹ which assign high likelihood to any 'natural' image of the world we live in,
- ² whose random samples have the 'look and feel' of natural images, i.e. make you look twice to see if you recognize something in them.

(三) QQ

[Field'87, Ruderman'94, Grenander & Srivastava'01...]

How to build stochastic image processes with non Gaussian statistics and a scale invariant behavior ? with some desirable properties like *homogeneity*, *isotropy*... E 2990

Examples

inserting an inhomogeneity

メロト メ部 トメ 君 トメ 君 トッ

 299

重

Physical interpretation

Several models use a distribution of elementary objects like the transported generator model by Grenander & Srivastava'01 or the model by Chi'98.

Compound Poisson Cascades can be interpreted as the superposition of transparent objects of random sizes:

$$
\log Q_{\ell}(\mathbf{x}) = \sum_{(\mathbf{x}_i,r_i) \in C_{\ell}(\mathbf{x})} \underbrace{\log W_i}_{\text{transparentcy}} \cdot \underbrace{f\left(\frac{\mathbf{x} - \mathbf{x}_i}{r_i}\right)}_{\text{object of size } r_i} + K
$$

- distribution of sizes $\propto \frac{1}{r^3}$
- **•** positions = Poisson point process (x_i, r_i)

[Matheron'68, Grenander'99, Huang & Mumford'99, Gousseau'01]... 2990

Capitalizing on machine learning

Expressivity of deep neural networks

▶ Deep learning

- strong expressivity
- very efficient for supervised learning
- large data set needed

Capitalizing on machine learning

Expressivity of deep neural networks

▶ Deep learning as a conference paper at ICLR 2021

- strong expressivity
- very efficient for supervised learning
- large data set needed

Capitalizing on machine learning

Expressivity of deep neural networks

▶ Deep learning

- strong expressivity
- very efficient for supervised learning
- large data set needed

GO TO ANIMATION

Sampling using normalizing flows (deep learning) F. Cœurdoux's PhD, N. Dobigeon - IRIT

(Deep) Learning changes of variables (optimal transport)

▶ MALAFlow: sampling in the Gaussian latent space

[Coeurdoux et al. \(2023\)](#page-59-0) preprint

Split Gibbs sampling (SGS) for inverse problems

Linear Gaussian inverse problems

 $y = Ax + n$

 $A =$ damaging operator (blur, binary mask...) $\mathbf{n} \sim \mathcal{N}\left(\mathbf{0}_{d}, \sigma^{2} \mathbf{I}_{d}\right) = \text{noise}.$

Posterior distribution
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp \left[-\frac{1}{2\sigma^2} ||\mathbf{y} - \mathbf{A}\mathbf{x}||_2^2 - \lambda g(\mathbf{x})\right]
$$

where $g(x) =$ prior knowledge on solutions.

- \bullet generally **high dimension** of the image, e.g. 1 million pixels,
- **2 generality** of the prior distribution of probability, cf. $g(x)$

Split Gibbs sampling (SGS)

Posterior distrib.

\n
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp\left[-\frac{1}{2\sigma^2}||\mathbf{y} - \mathbf{A}\mathbf{x}||_2^2 - \underbrace{\lambda g(\mathbf{x})}_{f_2(\mathbf{x})}\right]
$$
\n
$$
p(\mathbf{x}|\mathbf{y}) \propto \exp\left[-f_1(\mathbf{x}) - f_2(\mathbf{x})\right]
$$
\n
$$
\Downarrow
$$
\n
$$
\pi(\mathbf{x}, \mathbf{z}|\mathbf{x} = \mathbf{z}) \propto \exp\left[-f_1(\mathbf{x}) - f_2(\mathbf{z})\right] \text{ such that } \mathbf{x} = \mathbf{z}
$$
\n
$$
\Downarrow
$$
\n
$$
\pi_{\rho}(\mathbf{x}, \mathbf{z}) \propto \exp\left[-f_1(\mathbf{x}) - f_2(\mathbf{z}) - \frac{1}{2\rho^2}||\mathbf{x} - \mathbf{z}||_2^2\right]
$$

[Vono et al. \(2019a\)](#page-59-1)

Split Gibbs sampling (SP): conditional distributions

Full conditional distributions under the split distribution π_{ρ} :

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

$$
\pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto \exp\left(-f_2(\mathbf{z}) - \frac{1}{2\rho^2} ||\mathbf{x} - \mathbf{z}||_2^2\right)
$$

Note that f_1 and f_2 are now split in 2 distinct distributions "easy to use" thanks to state of the art sampling methods

[Vono et al. \(2019a\)](#page-59-1)

Split Gibbs sampling (SP): conditional distributions

Full conditional distributions under the split distribution π_{ρ} :

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

$$
\pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto \exp\left(-f_2(\mathbf{z}) - \frac{1}{2\rho^2} ||\mathbf{x} - \mathbf{z}||_2^2\right)
$$

Split Gibbs sampling (SP): conditional distributions

Full conditional distributions under the split distribution π_{ρ} :

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

$$
\pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto \exp\left(-f_2(\mathbf{z}) - \frac{1}{2\rho^2} ||\mathbf{x} - \mathbf{z}||_2^2\right)
$$

Split Gibbs sampling (SP): linear inverse problems

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

where

\n- $$
\blacktriangleright
$$
 H = forward operator
\n- \blacktriangleright **n** = noise with covariance Ω^{-1}
\n

Likelihood:

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

Splitted Gibbs sampling (SP): linear inverse problems

Full conditional distributions under the split distribution π_{ρ} :

$$
\begin{cases}\n\pi_{\rho}(\mathbf{x}|\mathbf{z}) \propto \exp\left[-\frac{f_1(\mathbf{x})}{q_{\text{uadratic}}}-\frac{1}{2\rho^2}\|\mathbf{x}-\mathbf{z}\|_2^2\right] \\
\pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto \exp\left[-\frac{f_2(\mathbf{z})}{2\rho^2}\|\mathbf{x}-\mathbf{z}\|_2^2\right] \\
\end{cases}
$$

Important notice: $\pi_{\rho}(z|x)$ is the posterior of a denoiser !

Splitted Gibbs sampling (SP): linear inverse problems

Full conditional distributions under the split distribution π_{ρ} :

$$
\begin{cases} \pi_{\rho}(\mathbf{x}|\mathbf{z}) \propto \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_{\mathbf{x}}, Q_{\mathbf{x}}^{-1}) \\ \pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto DDPM(t_n^*, \mathbf{z}|\mathbf{x}) \end{cases}
$$

Likelihood $=$ Gaussian distribution

$$
\begin{cases} \mathbf{Q}_{x} = \mathbf{H}^{T} \Omega \mathbf{H} + \frac{1}{\rho^{2}} \mathbf{I}_{N} \\ \mu_{x} = \mathbf{Q}_{x}^{-1} \left(\mathbf{H}^{T} \Omega \mathbf{y} + \frac{1}{\rho^{2}} \mathbf{z} \right) \end{cases}
$$

 $DDPM =$ Denoising Diffusion Probabilistic Model

Plug-and-Play and splitting: PnP-SGS F. Cœurdoux's PhD, N. Dobigeon

▶ PnP-SGS: using a deep denoiser as a prior in SGS

SGS uses Gibbs sampling from conditional posteriors

$$
\begin{cases}\n p(\mathbf{x} \mid \mathbf{y}, \mathbf{z}) \propto \exp\left[-f_1(\mathbf{y}, \mathbf{x}) - \frac{1}{2\rho^2} ||\mathbf{x} - \mathbf{z}||_2^2\right] \\
 p(\mathbf{z} \mid \mathbf{x}) \propto \exp\left[-f_2(\mathbf{z}) - \frac{1}{2\rho^2} ||\mathbf{x} - \mathbf{z}||_2^2\right]\n\end{cases}
$$

where $p(z | x) =$ posterior of a denoiser with reg. $\propto f_2(z)$

⇓

use a stochastic denoiser to sample from z

DDPM: Denoising Diffusion Probabilistic Models

The forward diffusion process adds noise from $t - 1$ to t:

$$
p(\mathbf{u}_t | \mathbf{u}_{t-1}) = \mathcal{N}\left(\mathbf{u}_t; \sqrt{1 - \beta(t)} \mathbf{u}_{t-1}, \beta(t) \mathbf{I}\right)
$$

Learn the backward SDE denoiser from t to $t - 1$:

$$
q_{\theta}\left(\mathbf{u}_{t-1} \mid \mathbf{u}_{t}\right) = \mathcal{N}\left(\mathbf{u}_{t-1}; \boldsymbol{\mu}_{\theta}\left(\mathbf{u}_{t}, t\right), \boldsymbol{\Sigma}_{\theta}\left(\mathbf{u}_{t}, t\right)\right)
$$

PnP-SGS using a DDPM

▶ Deep learning

- strong expressivity
- very efficient for supervised learning
- large data set needed

PnP-SGS using a DDPM

Starting from noise-free image \mathbf{u}_0 :

$$
\rho\left(\mathbf{u}_{t} \mid \mathbf{u}_{0}\right) = \mathcal{N}\left(\mathbf{u}_{t}; \sqrt{\bar{\alpha}(t)} \mathbf{u}_{0}, \alpha(t)\mathbf{I}\right)
$$

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

 \Rightarrow Gaussian noise with variance $\alpha(t^*)$

$$
p(z | \mathbf{x}) \propto \exp\left[-\frac{f_2(z)}{2\rho^2} \left\|\mathbf{x} - \mathbf{z}\right\|_2^2\right]
$$

= Gaussian denoiser

 \implies z = backward process from $u_{t^*} = x \implies p(z | x)$

PnP-SGS using a DDPM

Remarks:

- ▶ noise level $\alpha(t^*) \iff$ unique instant t^*
- ▶ the larger t^* , the noisier the image z_{t^*} .

Given a current sample $\mathbf{x}^{(n)}$ of SGS with noise level σ_n^2

$$
t^* = \alpha^{-1} \widehat{(\sigma_n^2)}
$$

using any good conventional estimator $\sigma^2 = \Phi(\mathbf{x}^{(n)})$

► larger
$$
t^*
$$
 ⇒ higher regularization

[\(Donoho and Johnstone 1994;](#page-59-2) [Guo et al. 2021;](#page-59-3) [Li et al. 2022\)](#page-59-4)

Inpainting task Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT

Original image - noisy masked - PnP-ADMM - PnP-SGS - 90% cred. int.

Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT original image

Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT noisy masked image

Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT PnP-SGS MMSE

Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT original image

Plug-and-Play and splitting: PnP-SGS - F. Cœurdoux's PhD, N. Dobigeon - IRIT 90% credibility intervals (PnP-SGS)

Inpainting task: comparisons on FFHQ

Runtime for each algorithm in Wall-clock time (computed with a single GTX 2080Ti GPU).

Inpainting task on FFHQ 256 \times 256 & Imagenet images FFHQ (2 top rows) and Imagenet (2 bottom rows)

FFHQ 256 \times 256 data set: image reconstruction

FFHQ 256 \times 256 data set: image reconstruction

Imagenet 256×256 data set: image reconstruction

Imagenet 256×256 data set: image reconstruction

PnP-SGS: inference with uncertainty quantification Plug-and-Play and splitting: F. Cœurdoux's PhD, N. Dobigeon - IRIT

Efficient sampling for high dimensional problems

Nicolas Dobigeon, Florentin Cœurdoux, Maxime Vono

PnP-SGS: efficient sampling for inverse problems in high dimensions

- ▶ SGS & SPA split-and-augment strategy
	- Bayesian inference for complex models
	- large scale problems (big & tall)
	- confidence intervals
- ▶ Efficient algorithms for sampling: ULA, MALA, MYULA
	- acceleration of state-of-the-art sampling algorithms
	- distributed inference (privacy, distr. comput.)
- ▶ AXDA: unifying statistical framework
	- asymptotically exact: control parameter ρ
	- non-asymptotic theoretical guarantees
- ▶ Capitalizing on ML: trained denoisers
	- learning from representative samples
	- State-of-the-art performance

Prospects

▶ Motivations for PnP-SGS

- posterior distribution \rightarrow Bayesian + MCMC
- **quantify uncertainty**
- adapt to any likelihood thanks to splitting

▶ Distributed sampling: fast and scalable: SPMD

- localized operators [\(Thouvenin et al. 2023\)](#page-59-11)
- distributed computing
- ▶ Equivariance: of course!

 \blacktriangleright Theoretical guarantees under mild assumptions?

- Chan, S. H., Wang, X., and Elgendy, O. A. (2016), "Plug-and-play ADMM for image restoration: Fixed-point convergence and applications," IEEE Transactions on Computational Imaging, 3, 84–98.
- Chung, H., Kim, J., Mccann, M. T., Klasky, M. L., and Ye, J. C. (2023), "Diffusion Posterior Sampling for General Noisy Inverse Problems," in Proc. of Int. Conf. on Learning Representations.
- Coeurdoux, F., Dobigeon, N., and Chainais, P. (2023), "Learning Optimal Transport Between Two Empirical Distributions with Normalizing Flows," in Machine Learning and Knowledge Discovery in Databases, eds. Amini, M.-R., Canu, S., Fischer, A., Guns, T., Kralj Novak, P., and Tsoumakas, G., Cham: Springer Nature Switzerland, pp. 275–290.
- Donoho, D. L. and Johnstone, J. M. (1994), "Ideal spatial adaptation by wavelet shrinkage," Biometrika, 81, 425–455.
- Guo, X., Liu, F., and Tian, X. (2021), "Gaussian noise level estimation for color image denoising." J. Opt. Soc. Am. A, 38, 1150–1159.
- Kawar, B., Elad, M., Ermon, S., and Song, J. (2022), "Denoising diffusion restoration models," arXiv preprint arXiv:2201.11793.
- Li, Y., Liu, C., You, X., and Liu, J. (2022), "A Single-Image Noise Estimation Algorithm Based on Pixel-Level Low-Rank Low-Texture Patch and Principal Component Analysis," Sensors, 22, 8899.
- Song, Y., Shen, L., Xing, L., and Ermon, S. (2022), "Solving Inverse Problems in Medical Imaging with Score-Based Generative Models," in Proc. of Int. Conf. on Learning Representations.
- Thouvenin, P.-A., Repetti, A., and Chainais, P. (2023), "A Distributed Block-Split Gibbs Sampler with Hypergraph Structure for High-Dimensional Inverse Problems," Journal of Computational and Graphical Statistics, 0, 1–35.
- Vono, M., Dobigeon, N., and Chainais, P. (2019a), "Split-and-augmented Gibbs sampler - Application to large-scale inference problems," IEEE Transactions on Signal Processing, 67, 1648–1661.
- — (2019b), "Split-and-augmented Gibbs sampler—Application to large-scale inference problems," IEEE Transactions on Signal Processing, 67, 1648–1661.
- Zhang, K., Li, Y., Zuo, W., Zhang, L., Van Gool, L., and Timofte, R. (2021), "Plug-and-play image restoration with deep denoiser prior," IEEE Transactions on Pattern Analysis and Machine Intelligence, 44, 6360-6376.

AXDA : comparing SPA & ADMM

Connection between MAP and ADMM

By replacing Gibbs sampling steps by optimizations, ADMM appears:

$$
\mathbf{x}^{(t)} \in \arg\min_{\mathbf{x}} - \log p\left(\mathbf{x}|\mathbf{z}^{(t-1)}, \mathbf{u}^{(t-1)}; \rho\right)
$$

$$
\mathbf{z}^{(t)} \in \arg\min_{\mathbf{z}} - \log p\left(\mathbf{z}|\mathbf{x}^{(t)}, \mathbf{u}^{(t-1)}; \rho\right)
$$

$$
\mathbf{u}^{(t)} = \mathbf{u}^{(t-1)} + \mathbf{x}^{(t)} - \mathbf{z}^{(t)}
$$