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

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Collaborators



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Image deblurring



Image deblurring



Image inpainting



Image inpainting





Motivations

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

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

with maybe some additional options such as:

- privacy preserving
- distributed computing

Bayesian approach + Monte Carlo method + machine learning?

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Bayesian approach + Monte Carlo method + machine learning?

The usual toolbox of inference

Optimization:

- $\bullet \ \ {\rm problem} \Rightarrow \ {\rm loss} \ {\rm function}$
- efficient algorithms
- theoretical guarantees
- interpretability / functional analysis

Bayesian approaches:

- probabilitic models
- uncertainty quantification
- Machine learning (deep):
 - $\bullet \ \ \mathsf{adaptive} \Rightarrow \mathsf{relevant}$
 - 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
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Bayesian estimators

$$\underset{\hat{\mathbf{x}}}{\arg\min} \int L(\mathbf{x}, \hat{\mathbf{x}}) \pi(\mathbf{x}|\mathbf{y}) \mathrm{d}\mathbf{x}$$

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



Credibility regions 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 $\hat{\textbf{x}}$

- **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

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

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



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 $g(\mathbf{x}) = prior$ knowledge on solutions.

- 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

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Natural images as stochastic processes

Conjecture by D. Mumford & B. Gidas :

There exists simply described stochastic models for images :

- which assign high likelihood to any 'natural' image of the world we live in,
- 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.

∃ na



[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*...

Examples



inserting an inhomogeneity



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:

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

- distribution of sizes $\propto \frac{1}{r^3}$
- positions = Poisson point process (\mathbf{x}_i, r_i)

[Matheron'68, Grenander'99, Huang & Mumford'99, Gousseau'01]... 🛓 🔈 🔍

Capitalizing on machine learning

Expressivity of deep neural networks

Deep learning

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



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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) preprint

Split Gibbs sampling (SGS) for inverse problems

Linear Gaussian inverse problems

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

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



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 $g(\mathbf{x}) = \text{prior knowledge on solutions.}$

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

Split Gibbs sampling (SGS)

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

Vono et al. (2019a)

Split Gibbs sampling (SP): conditional distributions

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

$$\begin{aligned} \pi_{\rho}(\mathbf{x}|\mathbf{z}) &\propto \exp\left(-f_{1}(\mathbf{x}) - \frac{1}{2\rho^{2}} \|\mathbf{x} - \mathbf{z}\|_{2}^{2}\right) \\ \pi_{\rho}(\mathbf{z}|\mathbf{x}) &\propto \exp\left(-f_{2}(\mathbf{z}) - \frac{1}{2\rho^{2}} \|\mathbf{x} - \mathbf{z}\|_{2}^{2}\right) \end{aligned}$$

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)

Split Gibbs sampling (SP): conditional distributions

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

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



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



Split Gibbs sampling (SP): linear inverse problems

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

where

Likelihood:

$$p(\mathbf{y} \mid \mathbf{x}) \propto \exp\left[-\underbrace{\frac{1}{2}(\mathbf{H}\mathbf{x} - \mathbf{y})^T \Omega(\mathbf{H}\mathbf{x} - \mathbf{y})}_{f_1(\mathbf{x})}
ight]$$

Splitted Gibbs sampling (SP): linear inverse problems

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

$$\begin{cases} \pi_{\rho}(\mathbf{x}|\mathbf{z}) \propto \exp\left[-\underbrace{f_{1}(\mathbf{x})}_{\text{quadratic}} -\frac{1}{2\rho^{2}} \|\mathbf{x}-\mathbf{z}\|_{2}^{2}\right] \\ \pi_{\rho}(\mathbf{z}|\mathbf{x}) \propto \exp\left[-\underbrace{f_{2}(\mathbf{z})}_{\text{prior}} -\frac{1}{2\rho^{2}} \|\mathbf{x}-\mathbf{z}\|_{2}^{2}\right] \end{cases}$$

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

Splitted Gibbs sampling (SP): linear inverse problems

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

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

Likelihood = Gaussian distribution

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

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

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

where $p(\mathbf{z} \mid \mathbf{x}) = \text{posterior of a denoiser with reg.} \propto f_2(\mathbf{z})$

₩

use a stochastic denoiser to sample from z

DDPM: Denoising Diffusion Probabilistic Models

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

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

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

$$q_{ heta}\left(\mathsf{u}_{t-1} \mid \mathsf{u}_{t}
ight) = \mathcal{N}\left(\mathsf{u}_{t-1}; oldsymbol{\mu}_{ heta}\left(\mathsf{u}_{t}, t
ight), oldsymbol{\Sigma}_{ heta}\left(\mathsf{u}_{t}, t
ight)
ight)$$

PnP-SGS using a DDPM

Deep learning

- strong expressivity
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PnP-SGS using a DDPM

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

$$p(\mathbf{u}_t \mid \mathbf{u}_0) = \mathcal{N}\left(\mathbf{u}_t; \sqrt{\bar{\alpha}(t)}\mathbf{u}_0, \alpha(t)\mathbf{I}\right)$$

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

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

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

= Gaussian denoiser

 \implies **z** = backward process from **u**_{t*} = **x** \implies $p(\mathbf{z} \mid \mathbf{x})$

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 $\widehat{\sigma^2} = \Phi(\mathbf{x}^{(n)})$

(Donoho and Johnstone 1994; Guo et al. 2021; Li et al. 2022)

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).

Method	Wall-clock time (s)	Ref.
PnP-ADMM	3.63	Chan et al. (2016)
Score-SDE	36.71	Song et al. (2022)
DDRM	2.03	Kawar et al. (2022)
DPIR	4.18	Zhang et al. (2021)
SGS-ULA	218.90	Vono et al. (2019b)
MCG	80.10	Chung et al. (2023)
DPS	43.89	Chung et al. (2023)
PnP-SGS	13.81	(IEEE Trans. Image Proc. 2024)

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

		PnP-SGS	SPA	TV-ADMM	PnP-ADMM	DPIR	Score-SDE	DDRM	MCG	DPS
painting	PSNR ↑	32.59	24.09	22.03	8.41	24.41	13.52	9.19	21.57	25.23
	SSIM ↑	0.913	0.524	0.784	0.325	0.809	0.437	0.319	0.751	0.851
	FID ↓	37.36	71.12	181.56	123.61	52.73	76.54	69.71	29.26	38.82
5	LPIPS \downarrow	0.144	0.785	0.463	0.692	0.398	0.612	0.587	0.286	0.262
gr L	PSNR ↑	27.96	23.17	22.37	24.93	26.09	7.12	23.36	6.72	24.25
urri ssia	SSIM ↑	0.837	0.499	0.801	0.812	0.820	0.109	0.767	0.051	0.811
Deblı (Gaus	FID ↓	59.667	78.67	186.74	90.42	80.18	109.07	74.92	101.2	62.72
	LPIPS \downarrow	0.331	0.452	0.507	0.441	0.392	0.403	0.332	0.340	0.444
g (PSNR ↑	28.46	17.73	21.36	24.65	27.33	6.58	N/A	6.72	20.92
tion	SSIM ↑	0.828	0.211	0.751	0.825	0.814	0.102	N/A	0.055	0.808
eblu	FID ↓	60.01	103.87	152.39	89.08	78.95	292.28	N/A	310.5	56.08
	LPIPS \downarrow	0.294	0.446	0.508	0.405	0.386	0.657	N/A	0.702	0.389
vi	PSNR ↑	25.99	N/A	23.86	25.55	26.14	17.62	25.36	19.97	25.67
Superre (×4)	SSIM ↑	0.862	N/A	0.803	0.865	0.889	0.617	0.835	0.703	0.852
	$FID\downarrow$	58.82	N/A	110.64	66.52	63.98	96.72	62.15	87.64	52.82
	LPIPS \downarrow	0.279	N/A	0.428	0.353	0.319	0.563	0.294	0.520	0.337

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	FID ↓	60.01	103.87	152.39	89.08	78.95	29	
	□))	$LPIPS \downarrow$	0.294	0.446	0.508	0.405	<u>0.386</u>	0.
	С	PSNR ↑	<u>25.99</u>	N/A	23.86	25.55	26.14	1
	uperre $(\times 4)$	SSIM ↑	0.862	N/A	0.803	<u>0.865</u>	0.889	0.
		$FID\downarrow$	<u>58.82</u>	N/A	110.64	66.52	63.98	90
	0)	$LPIPS \downarrow$	0.279	N/A	0.428	0.353	0.319	0.

Imagenet 256 \times 256 data set: image reconstruction

		PnP-SGS	SPA	TV-ADMM	PnP-ADMM	DPIR	Score-SDE	DDRM	MCG	DPS
nting	PSNR ↑	25.22	23.14	20.96	8.39	22.08	18.62	14.29	19.03	18.90
	SSIM ↑	0.870	0.802	0.676	0.300	0.762	0.517	0.403	0.546	0.794
ipai	FID ↓	34.28	41.33	189.3	114.7	37.47	127.1	114.9	39.19	35.87
<u>_</u>	LPIPS \downarrow	0.297	0.323	0.510	0.677	0.448	0.659	0.665	0.414	0.303
n (n	PSNR ↑	21.76	21.08	19.99	21.81	21.81	15.97	22.73	16.32	24.25
urri ssia	SSIM ↑	0.701	0.577	0.634	0.669	0.612	0.436	0.705	0.441	0.811
eblu	FID ↓	64.12	98.78	155.7	100.6	98.1	120.3	63.02	95.04	64.72
<u> </u>	LPIPS \downarrow	0.399	0.537	0.588	0.519	0.499	0.667	0.427	0.550	0.444
urring tion)	PSNR ↑	21.47	20.49	20.79	21.98	22.49	7.21	N/A	5.89	24.92
	SSIM ↑	0.695	0.681	0.677	0.702	0.731	0.120	N/A	0.037	0.859
eblu	FID ↓	47.57	91.51	138.8	89.76	76.11	98.25	N/A	186.9	56.08
Ō)	LPIPS \downarrow	0.372	0.538	0.525	0.483	0.448	0.591	N/A	0.758	0.389
vi	PSNR ↑	24.33	N/A	22.17	23.75	24.30	12.25	24.96	13.39	25.67
Superre (×4)	SSIM ↑	0.772	N/A	0.679	0.761	0.769	0.256	0.790	0.227	0.752
	$FID\downarrow$	59.09	N/A	130.9	97.27	88.85	170.7	59.57	144.5	50.66
	$LPIPS \downarrow$	0.418	N/A	0.523	0.433	0.424	0.701	0.339	0.637	0.337

Imagenet 256 \times 256 data set: image reconstruction

		PnP-SGS	SPA	TV-ADMM	PnP-ADMM	DPIR	Score-S
ള	PSNR ↑	25.22	23.14	20.96	8.39	22.08	18.62
ntir	SSIM ↑	0.870	<u>0.802</u>	0.676	0.300	0.762	0.517
ipai	$FID\downarrow$	34.28	41.33	189.3	114.7	37.47	127.1
<u> </u>	$LPIPS\downarrow$	0.297	0.323	0.510	0.677	0.448	0.659
ng n)	PSNR ↑	21.76	21.08	19.99	<u>21.81</u>	21.81	15.97
urri. ssia	SSIM ↑	0.701	0.577	0.634	0.669	0.612	0.436
Deblı (Gau:	$FID\downarrow$	<u>64.12</u>	98.78	155.7	100.6	98.1	120.3
	$LPIPS\downarrow$	0.399	0.537	0.588	0.519	0.499	0.667
ng (PSNR ↑	21.47	20.49	20.79	21.98	22.49	7.21
Deblurri (motion	SSIM ↑	0.695	0.681	0.677	0.702	<u>0.731</u>	0.120
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	$LPIPS\downarrow$	0.372	0.538	0.525	0.483	0.448	0.591
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Superre $(\times 4)$	SSIM ↑	<u>0.772</u>	N/A	0.679	0.761	0.769	0.256
	$FID\downarrow$	<u>59.09</u>	N/A	130.9	97.27	88.85	170.7
	$LPIPS\downarrow$	<u>0.418</u>	N/A	0.523	0.433	0.424	0.701

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
 - $\bullet\,$ 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)
- distributed computing
- **Equivariance**: of course!

Theoretical guarantees under mild assumptions?

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AXDA : comparing SPA & ADMM

Connection between MAP and ADMM

By replacing Gibbs sampling steps by optimizations, ADMM appears:

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