Bayesian inference with learnt generative image priors encoded by neural networks

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Outline

Imaging inverse problems

- We are interested in an unknown image $x^\star \in \mathbb{R}^d$.
- We measure $y \in \mathrm{Y}$, related to $x^\star$ by some mathematical model.
- For example, in many imaging problems

$$y = Ax^\star + w,$$

  for some operator A that is poorly conditioned or rank deficient, and an unknown perturbation or "noise" w.
- The recovery of $x^\star$ from y is usually not well posed. Additional information is required in order to deliver meaningful solutions.

Mathematical imaging frameworks

- There are three main mathematical and computational frameworks for inference in imaging inverse problems:
  1. Applied analysis
  2. Bayesian statistics.
  3. Machine learning.
- These frameworks have complementary strengths and weaknesses.
- Our aim is a unifying framework of theory, methods, and algorithms that inherits the benefits of each approach.

The Bayesian statistical approach

- Model $x^\star$ as a realisation of a r.v. $\mathbb{x}$ on $\mathbb{R}^d$. Use the distribution of $\mathbb{x}$ to regularise the problem and promote expected properties.

- The observation y is a realisation of a r.v. $(\mathbb{y}|\mathbb{x} = x^\star)$.

- Inferences about $x^\star$ from y are derived from the joint distribution of $(\mathbb{x}, \mathbb{y})$ - specified via the decomposition $p(x, y) = p(y|x)p(x)$.

- This determines the posterior distribution, with density

$$p(x|y) = \frac{p(y|x)p(x)}{\int_{\mathbb{R}^d} p(y|\tilde{x})p(\tilde{x})\mathrm{d}\tilde{x}},$$

which models our beliefs about $\mathbb{x}$ after observing $\mathbb{y} = y$.

Bayesian computation

- A simple algorithm to compute probabilities and expectations w.r.t. $p(x|y)$ is the Unadjusted Langevin Algorithm (ULA), given by

$$X_{k+1} = X_k + \delta_k \nabla \log p(y|X_k) + \delta_k \nabla \log p(X_k) + \sqrt{2\delta_k} Z_{k+1}\,,$$

where $Z_{k+1} \sim \mathcal{N}(0, \mathrm{I}_d)$ and $(\delta_k)_{k\in\mathbb{N}}$ is a sequence of step-sizes.

- The samples generated by ULA can be used to compute Monte Carlo estimates of $\hat{x}_{MMSE}$ and perform advanced inferences.

- ULA is remarkably well understood and provably convergent under easily verifiable conditions on $p(x|y)$.

(The SDE underpinning ULA)

- Important side note: ULA arises from discrete-time approximations of the Langevin diffusion process

$$\boldsymbol{X}: \quad \mathrm{d}\boldsymbol{X}_t = \frac{1}{2}\nabla \log p(\boldsymbol{X}_t|y)\,\mathrm{d}t + \mathrm{d}W_t, \quad 0 \leq t \leq T, \quad \boldsymbol{X}(0) = x_0.$$

  where W is the Brownian motion on $\mathbb{R}^d$.

- When $x \mapsto p(x|y) \in \mathcal{C}^1$ with $x \mapsto \nabla \log p(x|y)$ Lipschitz continuous, X_t converges exponentially fast to $p(x|y)$ as $t \to \infty$.

- ULA stems from a basic Euler approximations of $\boldsymbol{X}$.

- We recommend to use an accelerated approximation of $\boldsymbol{X}$ for significantly faster convergence (see 10.1137/19M1283719).

Outline

Generative image priors encoded by neural networks

Here, we focus on Bayesian inference based on deep generative priors for problems with abundant training data available to describe $\mathbb{x}$:

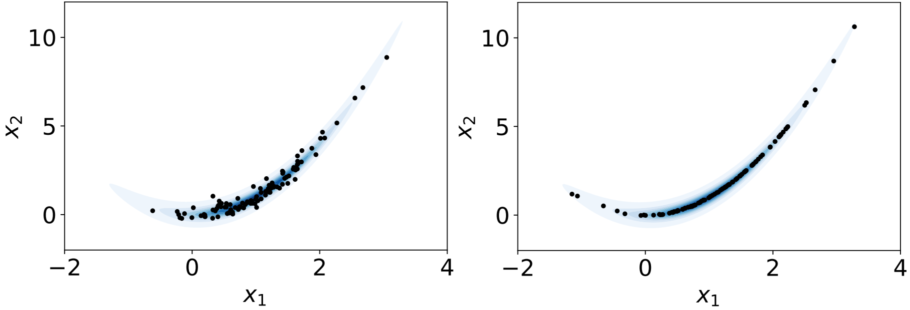
1. Let $\{x_i'\}_{i=1}^M$ be a training dataset that represents our prior knowledge about $\mathbb{x}$.

2. We adopt a manifold hypothesis and suppose that $\mathbb{x}$ takes values close to an unknown p-dimensional submanifold of $\mathbb{R}^d$.

3. To estimate the manifold, we introduce a latent r.v. $\mathbb{z}$ on $\mathbb{R}^p$, with $p \ll d$, and a mapping $\nu_\theta : \mathbb{R}^p \mapsto \mathbb{R}^d$, such that the push-forward measure of $\mathbb{z} \sim \mathcal{N}(0, \mathrm{I}_p)$ under ν_θ is close to $\{x_i'\}_{i=1}^M$ (in dist.).

4. We implement ν_θ as a neural network. Can learn ν_θ from $\{x_i'\}_{i=1}^M$ by using, e.g., a VAE, a GAN, or a normalising flow approach.

Illustrative example - Rosenbrock distribution



Left: training data from the two-dimensional Rosenbrock distribution. Right: push-forward of $\mathbb{z} \sim \mathcal{N}(0, \mathrm{I}_p)$ under ν_θ as implemented by a VAE, with $p = 1$.

Posterior distributions for generative priors

- With $\mathbb{z}$ and ν_θ, we have the likelihood $p(y|z) = p(y|x = \nu_\theta(z))$.
- We use Bayes' theorem to derive the posterior for $\mathbb{z}|\mathbb{y} = y$

$$p(z|y) = \frac{p(y|x = \nu_\theta(z))p(z)}{\int_{\mathbb{R}^p} p(y|\tilde{z})p(\tilde{z})\mathrm{d}\tilde{z}} \,,$$

- Pushing $(\mathbb{z}|\mathbb{y} = y)$ under $\nu_\theta(z)$ leads to the posterior for $(\mathbb{x}|\mathbb{y} = y)$, which supported on a manifold and does not have a density.

Key questions

Some fundamental questions:

1. Under what conditions on the generative model are the resulting Bayesian models well-posed and amenable to efficient computation? Do the key quantities of interest inherit this well-posed nature?
2. Are these Bayesian methods and algorithms delivering solutions that are meaningful from a non-subjective point of view?
3. Can we guarantee the convergence of ULA under easily verifiable conditions, with non-asymptotic accuracy bounds?

In this short talk, we will focus on the first two questions and demonstrate the approach with some numerical experiments.

Key papers

For technical details please see:

1. M. Holden, M. Pereyra, K. Zygalakis, "Bayesian Imaging with Data-Driven Priors Encoded by Neural Networks", SIAM Journal on Imaging Sciences, 15 (2), 2022. `https://doi.org/10.1137/21M1406313`.

2. S. Melidonis, M. Holden, M. Pereyra, K. Zygalakis, "Empirical Bayesian imaging with conditional generative priors encoded by neural networks", in preparation.

The oracle Bayesian model

We analyse Bayesian models with data-driven priors in an *M-complete* modelling framework:

- There exists a true - albeit unknown - marginal distribution for $\mathbb{x}$ and posterior distribution for $(\mathbb{x}|\mathbb{y} = y)$.

- Basing inferences on these oracle models is theoretically optimal.

- We henceforth denote this optimal prior distribution by μ. When μ admits a density w.r.t. the Leb. measure on $\mathbb{R}^d$, we denote it by $p^\star$.

- In that case, the posterior for $x|y$ has density

$$p^\star(x|y) = \frac{p(y|x)p^\star(x)}{\int_{\mathbb{R}^d} p(y|\tilde{x})p^\star(\tilde{x})\mathrm{d}\tilde{x}}\,.$$

The oracle Bayesian model

We analyse Bayesian models with data-driven priors in an *M-complete* modelling framework:

- Conceptual construction: μ naturally depends on the application.
- We regard the training data $\{x'_i\}_{i=1}^M$ as a sample from μ.
- When we learn ν_θ and approximate μ by assuming that $\mathbb{x} = \nu_\theta(\mathbb{z})$ for $\mathbb{z} \sim \mathcal{N}(0, \mathrm{I}_p)$, pushing $(\mathbb{z}|\mathbb{y} = y)$ under ν_θ leads to the posterior for $(\mathbb{x}|\mathbb{y} = y)$ that approximates the oracle $p^\star(x|y)$.
- Holden et al. (2022a) establishes that $(\mathbb{z}|\mathbb{y} = y)$ and $(\mathbb{x}|\mathbb{y} = y)$ are well-posed in the sense of Hadamard and have finite moments.

Outline

Illustrative experiments

- We first illustrate the proposed approach with the MNIST dataset.
- We perform the following advanced inferences:
  1. Identify the latent dimension p.
  2. Perform MMSE inference in challenging image denoising, inpainting, and deblurring experiments.
  3. Adopt a likelihood-ratio test to detect out-of-sample observations that should not be analysed with the Bayesian model.
  4. Assess the frequentist accuracy of the Bayesian probabilities reported by the model.
- We report comparisons with MAP estimation under the same model, and with PnP-ADMM by using a DnCNN denoiser.

Identification of manifold dimension p

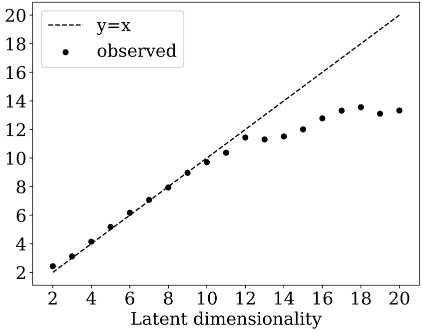
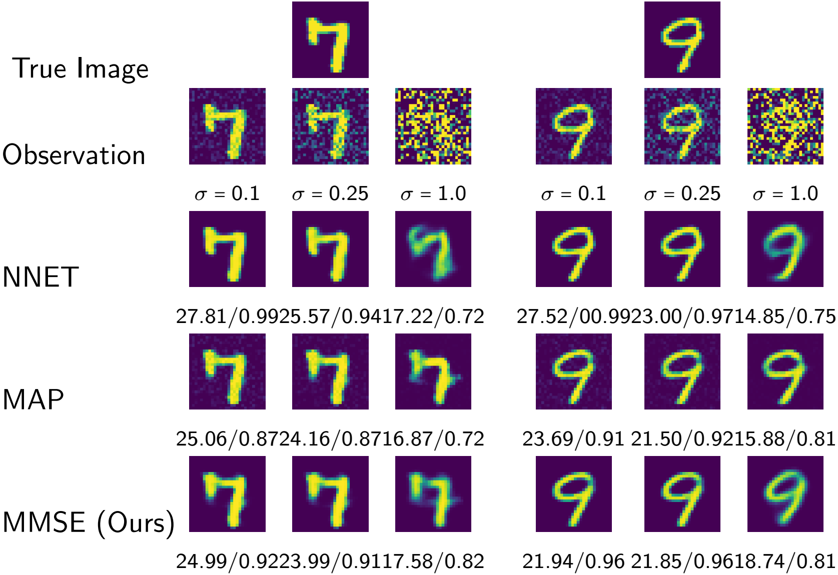
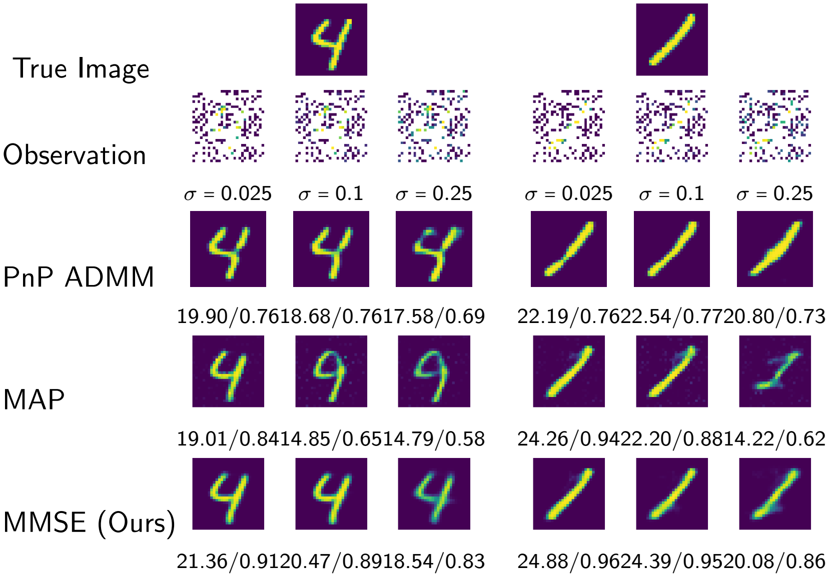


Figure: Trace of sample covariance of $\nu_\theta(x_i)$ across all test images. The amount of information encoded by the prior stabilises for $p \approx 12$, additional dimensions do not significantly increase the amount of prior information encoded .

Denoising

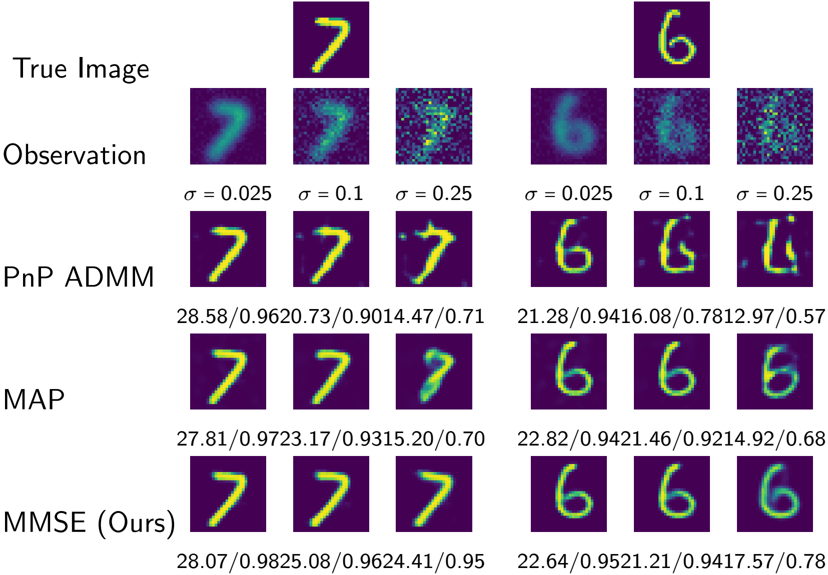

True Image
Observation
$\sigma = 0.1$ $\sigma = 0.25$ $\sigma = 1.0$ $\sigma = 0.1$ $\sigma = 0.25$ $\sigma = 1.0$
NNET
27.81/0.9925.57/0.9417.22/0.72 27.52/00.9923.00/0.9714.85/0.75
MAP
25.06/0.8724.16/0.8716.87/0.72 23.69/0.91 21.50/0.9215.88/0.81
MMSE (Ours)
24.99/0.9223.99/0.9117.58/0.82 21.94/0.96 21.85/0.9618.74/0.81

Inpainting



True Image
Observation
σ = 0.025
σ = 0.1
σ = 0.25
σ = 0.025
σ = 0.1
σ = 0.25
PnP ADMM
19.90/0.7618.68/0.7617.58/0.69
22.19/0.7622.54/0.7720.80/0.73
MAP
19.01/0.8414.85/0.6514.79/0.58
24.26/0.9422.20/0.8814.22/0.62
MMSE (Ours)
21.36/0.9120.47/0.8918.54/0.83
24.88/0.9624.39/0.9520.08/0.86

Deconvolution



Likelihood ratio test for out-of-distribution detection

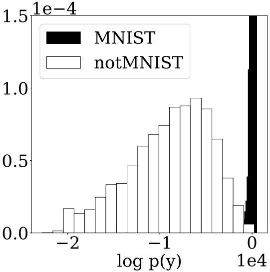


Figure: Denoising

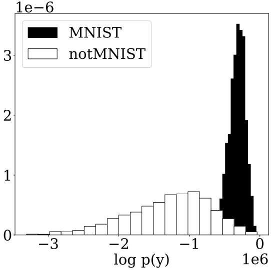


Figure: Inpainting

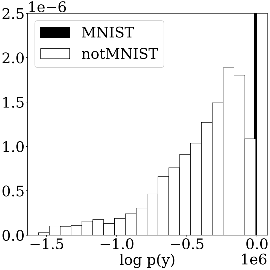


Figure: Deblurring

Figure: Histograms of marginal likelihoods for image denoising, inpainting and deblurring experiments. Out-of-sample detection powers for notMNIST of 99.6%, 88.5% and 99.8% respectively.

Coverage test: frequentist accur. of Bayesian probabilities

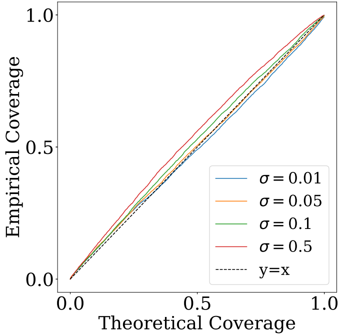


Figure: Denoising

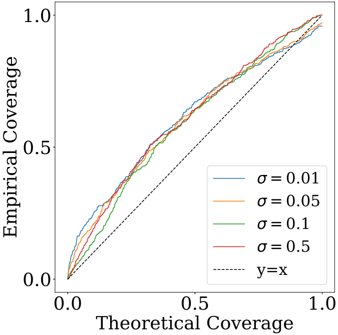
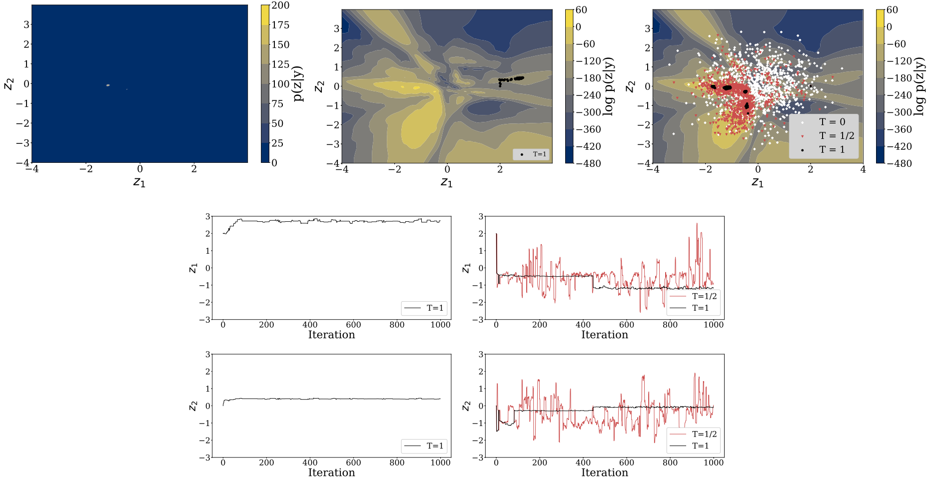


Figure: Inpainting

Multimodality? Use temperatures..

Toy example in dimension $p = 2$: three interacting Markov chains targeting $p_T(z|y) \propto p(y|z)^T p(z)$ for $T = \{0, 0.5, 1\}$.



Outline

Conditional generative priors

- Despite their success in computer vision, scaling generative models to large inference problems reliably is difficult because of mode collapse, spurious modes, or other sources of bias.

- To reduce the difficulty of the machine learning problem, we consider a conditional generative model $\mathbb{x} = \nu_\theta^u(\mathbb{z})$, $\mathbb{z} \sim \mathcal{N}(0, \mathrm{I}_p)$, that models the distribution of $\mathbb{x}$ given some additional r.v. $\mathbb{u} = u$.

- For example, we let $\mathbb{u}$ denote a low resolution version of $\mathbb{x}$, and implement ν_θ^u by using a normalising flow for image super-resolution.

- This leads to the model

$$p(z|y, u) = \frac{p(y|z, u)p(z)}{p(y|u)}\,,$$

with $p(y|z, u) = p(y|x = \nu_\theta^u(z))$ and $p(y|u) = \int_{\mathbb{R}^p} p(y|\tilde{z}, u)p(\tilde{z})\mathrm{d}\tilde{z}$.

Empirical Bayesian imaging with conditional generative priors

- We accurately estimate $u^\star$ from y by maximum marginal likelihood estimation:

$$\hat{u} = \underset{\mu}{\operatorname{argmax}}\, p_\theta(y|u)\,.$$

- Adopting an empirical Bayesian strategy, we perform inference on $(\mathbb{x}|\mathbb{y} = y, \mathbb{u} = \hat{u})$ by using

$$p(z|y, \hat{u}) = \frac{p(y|z, \hat{u})p(z)}{p(y|\hat{u})}\,,$$

  and pushing to $(\mathbb{z}|\mathbb{y} = y, \mathbb{u} = \hat{u})$ via ν_θ^u.

- This can be performed computationally efficiently by using ULA within a Stochastic Approximation Proximal Gradient scheme that simultaneously computes $\hat{u}$ and draws samples from $(\mathbb{z}|\mathbb{y} = y, \mathbb{u} = \hat{u})$. See `https://doi.org/10.1007/s11222-020-09986-y` and `https://doi.org/10.1137/20M1339829` for details.

Illustrative example - Image deblurring

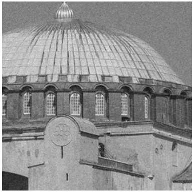
We compare the MMSE estimator obtained with the proposed method and the MAP-style estimator obtained from PnP-ADMM, by using a DnCNN end-to-end denoising prior, on an image deblurring problem.

$x^\star$ | y | PnP-ADMM | Proposed

Figure: Image deblurring experiment: 9×9 uniform blur, $\sigma = 10$.

Illustrative example - Image pan-sharpening

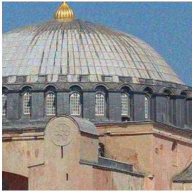
We seek to recover $x^\star$ from two noisy linear observations y_1 and y_2, one with spectral fine details and the other with spatial fine detail.



y_1

y_2

Proposed (31.5dB)



PnP ADMM (28.5dB)

$x^\star$

Outline

Conclusion

- We have studied methodology for Bayesian inference with generative priors encoded by neural networks, learnt from training data.
- We rooted our study in the Bayesian *M-complete* paradigm that views generative Bayesian models as approximations of an oracle model.
- A key challenge to scale the approach to large problems is that generative models struggle to learn high-dimensional distributions.
- We have addressed that difficulty by adopting an empirical Bayesian approach and considering a conditional generative prior.

Thank you!