Bayesian Inversion for Nonlinear Imaging Models using Deep Generative Priors

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Abstract-Most modern imaging systems involve a computational reconstruction pipeline to infer the image of interest from acquired measurements. The Bayesian reconstruction framework relies on the characterization of the posterior distribution, which depends on a model of the imaging system and prior knowledge on the image, for solving such inverse problems. Here, the choice of the prior distribution is critical for obtaining highquality estimates. In this work, we use deep generative models to represent the prior distribution. We develop a posterior sampling scheme for the class of nonlinear inverse problems where the forward model has a neural-network-like structure. This class includes most existing imaging modalities. We introduce the notion of augmented generative models in order to suitably handle quantitative image recovery. We illustrate the advantages of our framework by applying it to two nonlinear imaging modalities-phase retrieval and optical diffraction tomography.

Index Terms—Bayesian inference, nonlinear inverse problems, phase retrieval, optical diffraction tomography, neural networks, generative models, generative adversarial networks

I. Introduction

In practical imaging systems, the object of interest $\mathbf{s} \in \mathbb{R}^K$ is observed indirectly by performing a series of measurements $\mathbf{v} \in \mathbb{C}^M$. Mathematically, this process is modelled as

$$\mathbf{y} = \mathbf{H}\{\mathbf{s}\} + \mathbf{n},\tag{1}$$

where $\mathbf{H}: \mathbb{R}^K \to \mathbb{C}^M$ is an operator that describes the physics of the imaging system and $\mathbf{n} \in \mathbb{C}^M$ is an additive noise. The operator \mathbf{H} can be linear or nonlinear depending on the imaging modality. For example, in magnetic resonance imaging (MRI), one captures noisy samples of the Fourier transform of the signal. The task at hand is then to reconstruct the signal s from the obtained measurements \mathbf{y} . Typically, such inverse problems are ill-posed in the sense that there exist several signals which produce similar measurements. Thus, we cannot rely on direct inversion techniques to obtain relevant solutions.

A. Variational Methods

In variational methods, the solution to the inverse problem is specified as the minimizer of a cost functional

$$\widehat{\mathbf{s}} = \underset{\mathbf{s} \in \mathbb{R}^K}{\operatorname{arg\,min}} \left(E(\mathbf{y}, \mathbf{H}\{\mathbf{s}\}) + \lambda R(\mathbf{s}) \right), \tag{2}$$

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where the data-fidelity term $E: \mathbb{C}^M \times \mathbb{C}^M \to \mathbb{R}_+$ forces the solution to be consistent with the measurements, the regularization $R: \mathbb{R}^K \to \mathbb{R}_+$ imposes some prior knowledge about the signal of interest on the solution and $\lambda \in \mathbb{R}_+$ is a tunable hyperparameter. Typical candidates for these terms are $E(y, H\{s\}) = ||y - H\{s\}||_2^2$ and $R(s) = ||Ls||_p^p$ [1]-[7] with $p \in [1,2]$. Here, L is a linear transformation such as the discrete version of the wavelet transform or the gradient operator, that takes part in the regularization. The well-known total-variation (TV) regularization [3] which uses the ℓ_1 -norm along with the gradient operator promotes solutions with sparse derivatives. It is widely used for compressed sensing and extreme imaging applications where the data is scarce [7]. The resulting optimization problems are typically solved by iterative algorithms such as gradient descent, FISTA [8] or ADMM [9].

B. Bayesian Inference

In the Bayesian approach to image reconstruction for solving inverse problems [10]–[13], the signal s is modelled as a realization of a random vector with a suitable probability density function (pdf) p_S that captures our prior knowledge about the signal. The idea here is to characterize the posterior distribution

$$p_{S|Y}(\mathbf{s}|\mathbf{y}) \propto p_N(\mathbf{y} - \mathbf{H}\{\mathbf{s}\})p_S(\mathbf{s}),$$
 (3)

which depends on the statistics of the noise p_N and the prior distribution p_S , and make inferences based on it.

The posterior distribution can be used for the derivation of several point estimators for the signal \mathbf{s} . One such example is the maximum a posteriori (MAP) estimator, which is the mode of the posterior distribution. The MAP estimator leads to an optimization problem that resembles (2), with $E(\mathbf{y}, \mathbf{H}\{\mathbf{s}\}) \propto \left(-\log\left(p_N(\mathbf{y}-\mathbf{H}\{\mathbf{s}\})\right)\right)$ and $R(\mathbf{s}) \propto \left(-\log\left(p_S(\mathbf{s})\right)\right)$, and thus links the variational and Bayesian approaches [14]–[16]. Another example is the minimum mean square error (MMSE) estimator which turns out to be the posterior mean.

Besides the derivation of point estimators, the Bayesian framework further allows us to quantify the uncertainty of the reconstructed image. This feature addresses an important challenge in computational imaging as sophisticated reconstruction algorithms, such as the variational methods, often lack reliability assessment.

In general, performing such inference tasks entails the estimation of expected values with respect to the posterior distribution. Typically, these are high-dimensional integrals that cannot be evaluated analytically. Thus, one relies on

Markov Chain Monte Carlo (MCMC) methods to efficiently draw samples from the posterior and then uses them to approximate the integrals [17]–[20].

C. Deep Learning Based Methods

Over the past few years, researchers have started deploying deep-learning-based methods for solving inverse problems in imaging. The learning-based methods have been found to outperform the traditional model-based ones. Broadly speaking, their underlying principle is to utilize large amounts of training data to improve the reconstruction quality instead of prespecifying prior information about the image of interest in the form of mathematical models, as in the variational and Bayesian approaches described earlier.

The first generation of deep-learning-based methods involve training a convolutional neural network (CNN) as a nonlinear mapping that relates a low-quality estimate of the signal to the desired high-quality estimate [21]–[25]. The reconstruction pipeline then consists of using a fast classical algorithm to yield an initial solution and then correcting for its artifacts using the trained CNN. This category of methods includes "unrolling" [26]–[31], where the architecture of the CNN is designed by studying iterations of algorithms used for solving Problem (2). While these first generation end-to-end learning methods have achieved state-of-the-art performances in several inverse problems, recent works have highlighted their instability and lack of robustness [32], [33].

The second generation of deep-learning-based methods aim to integrate CNNs into iterative reconstruction algorithms. The Plug-and-Play priors (PnP) [34] and Regularization-by-Denoising (RED) [35] frameworks are two successful examples that provide a way to carry out this integration. In PnP algorithms, the proximal operator appearing in iterations of proximal algorithms (FISTA, ADMM) is replaced by a generic denoiser which represents an implicit prior on the signal. RED, by contrast, incorporates an explicit regularization term that is constructed with the help of the chosen denoiser. In the learning-based variants of these frameworks, one uses appropriately trained CNNs as the denoising routines [36]-[42]. Another example of such methods is projected gradient descent where the projection operator is a trained neural network that projects onto the space of desired signals [43]–[45]. Unlike the first generation methods, the second generation ones enforce consistency between the reconstructed signal and the acquired measurements. They are also more versatile as the CNN denoisers can be used for different kinds of inverse problems without the need for retraining. The difficulty in employing these learning-based iterative schemes is that the Lipschitz constant of the CNNs must be controlled in order to ensure their convergence [46], [47], which is not straightforward and remains an active area of research [47]-[49].

Finally, we also mention a third class of deep-learning-based methods that make use of deep generative models such as variational autoencoders (VAE) [50] and generative adversarial networks (GAN) [51]. These models consist of generator networks that map a low-dimensional latent space to

the high-dimensional signal space. They are trained to capture the statistics of the dataset and generate sample signals similar to those in the dataset. Once a deep generative model has been successfully trained, its application to an inverse problem typically consists of finding the optimal latent variable such that the resulting signal best fits the measurements. Recent works have focused on designing and analyzing algorithms for the task of inverting generative models [52]–[55].

The three classes of deep-learning-based methods that we have discussed so far are variational in nature and they provide a single reconstruction as the output. Given the success of these methods, there has naturally been interest in developing Bayesian methods that exploit the power of neural networks. This has led to the development of various posterior sampling schemes for priors that are defined either implicitly through denoising CNNs (like the ones used in the PnP or RED frameworks) [56]–[58] or through generative models such as GANs and VAEs [59]–[61]. So far, most works have focused on inverse problems with linear or linearized forward models.

A current frontier in imaging is the inversion of nonlinear models, which arise in several applications, with two notable examples being phase retrieval and optical diffraction tomography. Such applications could benefit greatly from the development of neural-network-based Bayesian reconstruction methods.

D. Contributions

The goal of this paper is to present a Bayesian framework for solving a broad class of nonlinear inverse problems, where the prior on the image of interest is represented by a trained deep generative model. Our contributions are as follows.

- We develop a method based on the Metropolis-adjusted Langevin Algorithm (MALA) [62], [63] to sample from the posterior distribution for the class of nonlinear inverse problems where the forward model has a neural-networklike structure. This class includes a wide variety of practical imaging modalities. We show that the structure of the forward model and the low-dimensional latent space of the generative prior enable tractable Bayesian inference.
- We introduce the concept of augmented generative models. This is motivated by the observation that deep generative models are easier to train when the dataset consists of images with the same range of pixel values. Unfortunately, such models are not well-matched to imaging modalities where one is interested in extracting the absolute intensity of objects rather than visualizing contrast. Our proposed augmented models provide us with a simple but effective way of overcoming the aforementioned problem.
- We illustrate the advantages of the proposed reconstruction framework with the help of numerical experiments for two nonlinear imaging modalities - phase retrieval and optical diffraction tomography.

II. NONLINEAR INVERSE PROBLEMS: FORWARD MODELS

In this section, we first briefly describe the class of nonlinear inverse problems that we are interested in. We then focus on

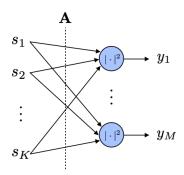


Fig. 1: The forward model for phase retrieval (6) expressed as a one-layer fully-connected neural network with linear weights **A** and quadratic activation functions.

two concrete examples—phase retrieval and optical diffraction tomography—and detail the physical models involved.

A. Nonlinear Inverse Problems

The objective is to recover an image $\mathbf{s} \in \mathbb{R}^K$ from its noisy measurements $\mathbf{y} \in \mathbb{C}^M$ given by

$$\mathbf{y} = \mathbf{H}\{\mathbf{s}\} + \mathbf{n},\tag{4}$$

where $\mathbf{H}: \mathbb{R}^K \to \mathbb{C}^M$ is a nonlinear operator that models the physics of the imaging system and $\mathbf{n} \in \mathbb{C}^M$ is additive noise. In this work, we consider the class of nonlinear inverse problems where the computational structure of the forward model \mathbf{H} is a directed acyclic graph and thus resembles a neural network.

The Jacobian matrix of **H** at any point $\mathbf{x} = (x_1, \dots, x_K) \in \mathbb{R}^K$ is defined as

$$\mathbf{J}_{\mathbf{H}}(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} [\mathbf{H} \{ \mathbf{x} \}]_1 & \cdots & \frac{\partial}{\partial x_K} [\mathbf{H} \{ \mathbf{x} \}]_1 \\ \vdots & \vdots & \vdots \\ \frac{\partial}{\partial x_1} [\mathbf{H} \{ \mathbf{x} \}]_M & \cdots & \frac{\partial}{\partial x_K} [\mathbf{H} \{ \mathbf{x} \}]_M \end{bmatrix}. \quad (5)$$

Gradient-based MCMC methods (see Section III for a specific example) involve computing quantities such as $\mathbf{J}_{\mathbf{H}}^{H}(\mathbf{x})\mathbf{r}$ for some vectors $\mathbf{x} \in \mathbb{R}^{K}$, $\mathbf{r} \in \mathbb{C}^{M}$, and this can be a potential bottleneck. The neural-network-like structure of \mathbf{H} allows us to compute these efficiently using the error backpropagation algorithm. This, in turn, makes tractable Bayesian inference computationally feasible.

The class of nonlinear inverse problems that fit this description is very broad and adaptable to most existing imaging modalities. In principle, it covers all possible inverse problems. The linear case is trivially covered. More generally, if sufficient data is available, one can rely on the universal approximation property of neural networks and train such a system to mimic the physics of our forward model. Next, we look at two particular problems that fall within this class that we have defined.

B. Phase Retrieval

Phase retrieval [64], [65] is a prevailing nonlinear inverse problem that is ubiquitous in computational imaging. The aim

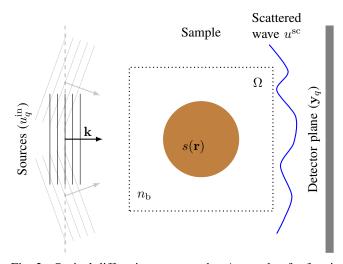


Fig. 2: Optical diffraction tomography. A sample of refractive index $n_b + s(\mathbf{r})$ is immersed in a medium of index n_b and illuminated by an incident plane wave (wave vector \mathbf{k}). The interaction of the wave with the object produces scattered waves, which are recorded at the detector plane.

there is to recover a signal from its intensity-only measurements which is a central issue in optics [66], [67], astronomy [68], [69] and computational microscopy [70]–[73].

In the phase retrieval problem that we consider in this paper, the measurements are modelled as

$$\mathbf{y} = \mathbf{H}_{\text{pr}}\{\mathbf{s}\} + \mathbf{n} = |\mathbf{A}\mathbf{s}|^2 + \mathbf{n},\tag{6}$$

where $\mathbf{A}: \mathbb{R}^K \to \mathbb{C}^M$ is either the Fourier matrix [66], [73], [74] or a fixed random matrix with independent and identically distributed (i.i.d.) elements [65], [75], [76], and $|\cdot|^2$ is a component-wise operator. As shown in Figure 1, the forward model in (6) can be expressed as a one-layer fully-connected neural network with fixed linear weights \mathbf{A} and quadratic activation functions.

C. Optical Diffraction Tomography

In optical diffraction tomography (ODT), the aim is to recover the refractive index (RI) map of a sample from complex-valued measurements of the scattered fields generated when the sample is probed by a series of tilted incident fields [77]. According to the scalar diffraction theory, the propagation of the incident fields through the sample is governed by the wave equation. While pioneering works relied on linear models to approximate the field propagation [77], [78], recent works have significantly improved the quality of RI reconstruction by using more accurate nonlinear models which account for multiple scattering [79]. Here, we look at one such nonlinear model called the Beam Propagation Method (BPM).

Helmholtz Equation: We consider a sample with a real-valued spatially varying refractive index that is immersed in a medium with refractive index n_b , as shown in Figure 2. The refractive index distribution in our region of interest $\Omega = [0, L_x] \times [0, L_z]$ is represented as $n(\mathbf{r}) = n_b + s(\mathbf{r})$, where

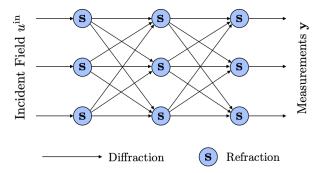


Fig. 3: The computational structure for BPM that resembles a neural network.

 $\mathbf{r}=(x,z)$ and $s(\mathbf{r})$ is the refractive index contrast. The sample is illuminated with an incident plane wave $u^{\mathrm{in}}(\mathbf{r})$ of free space wavelength λ , whose direction of propagation is specified by the wave vector \mathbf{k} . The total field $u(\mathbf{r})$ resulting from the interaction between the sample and the incident wave is then recorded at certain positions $\{\mathbf{r}_m\}_{m=1}^{M'}$ in the detector plane Γ to yield complex measurements $\mathbf{y} \in \mathbb{C}^{M'}$. The interplay between the total field $u(\mathbf{r})$ at any point in space and the refractive index contrast $\delta n(\mathbf{r})$ is described by the Helmholtz equation

$$\nabla^2 u(\mathbf{r}) + k_0^2 n^2(\mathbf{r}) u(\mathbf{r}) = 0, \tag{7}$$

where $k_0 = \frac{2\pi}{\lambda}$.

Beam Propagation Method: For computational purposes, the region of interest Ω is subdivided into a $N_x \times N_z$ array of pixels with sampling steps δ_x and δ_z , respectively. The corresponding samples of the refractive index contrast $s(\mathbf{r})$ and total field $u(\mathbf{r})$ are stored in the vectors $\mathbf{s} \in \mathbb{R}^K$ and $\mathbf{u}^1 \in \mathbb{C}^K$, respectively, where $K = N_x N_z$. Further, let $\mathbf{s}_k \in \mathbb{R}^{N_x}$ and $\mathbf{u}_k \in \mathbb{C}^{N_x}$ represent the above quantities when restricted to the slice $z = k\delta_z$.

The beam propagation method (BPM) computes the total field ${\bf u}$ in a slice-by-slice manner along the z-axis. For a given incident wave $u^{\rm in}({\bf r})$ that is propagated over a region larger than Ω , we set the initial conditions as ${\bf u}_{-1}({\bf s})=\left(u^{\rm in}(x=i\delta_x,z=-\delta_z)\right)_{i=0}^{N_x-1}\in\mathbb{C}^{N_x}$. The total field over Ω is then computed via a series of diffraction and refraction steps

$$\widetilde{\mathbf{u}}_k(\mathbf{s}) = \mathbf{u}_{k-1}(\mathbf{s}) * \mathbf{h}_{\text{DTOD}}^{\delta_z}$$
 (diffraction) (8)

$$\mathbf{u}_k(\mathbf{s}) = \widetilde{\mathbf{u}}_k(\mathbf{s}) \odot \mathbf{p}_k(\mathbf{s})$$
 (refraction), (9)

where $k=0,1,\ldots,N_z-1$. The convolution kernel $\mathbf{h}_{\mathrm{prop}}^{\delta_z} \in \mathbb{C}^{N_x}$ for the diffraction step is characterized in the Fourier domain as

$$\mathcal{F}\left\{\mathbf{h}_{\text{prop}}^{\delta_z}\right\} = e^{\mathrm{j}\delta_z \left(\sqrt{k_0^2 n_b^2 - \mathbf{w}_x^2}\right)},\tag{10}$$

where \mathcal{F} denotes the discrete Fourier transform and $\mathbf{w}_x \in \mathbb{R}^{N_x}$ is the frequency variable. The subsequent refraction step

involves a pointwise multiplication with the phase mask

$$\mathbf{p}_k(\mathbf{s}) = e^{jk_0 \delta_z \mathbf{s}_k}. (11)$$

Finally, we define an operator $\mathbf{R}: \mathbb{C}^{N_x} \mapsto \mathbb{C}^{M'}$ that propagates $\mathbf{u}_{N_z-1}(\mathbf{s})$ to the detector plane Γ and restricts it to the sensor positions to give us the measurements $\mathbf{y} \in \mathbb{C}^{M'}$. Thus, for a given incident wave u^{in} , our nonlinear BPM forward model is of the form

$$\mathbf{y} = \mathbf{H}_{bpm}(\mathbf{s}; u^{in}) + \mathbf{n} = \mathbf{R}(\mathbf{u}_{N_z - 1}(\mathbf{s})) + \mathbf{n}. \tag{12}$$

In Figure 3, we show the implementation of \mathbf{H}_{bpm} as a directed acyclic graph.

Complete Forward Model: We assume that the sample is illuminated with Q incident plane waves $\{u_q^{\rm in}\}_{q\in\{1,\dots,Q\}}$ and the corresponding measurements are $\{\mathbf{y}_q\in\mathbb{C}^{M'}\}_{q\in\{1,\dots,Q\}}$. These measurements are related to the RI variation \mathbf{s} of the sample through the BPM forward model in (12). We define a stacked measurement vector as $\mathbf{y}=[\mathbf{y}_1,\dots,\mathbf{y}_Q]\in\mathbb{R}^M$ (M=QM'). This allows us to rewrite the complete forward model in the form of (4) where the operator \mathbf{H} consists of applying $\mathbf{H}_{\mathrm{bpm}}$ with all the different illuminations and concatenating the outputs into a single vector.

III. BAYESIAN RECONSTRUCTION FRAMEWORK

We now present our reconstruction framework, which makes use of the prior statistical information, in order to solve the generic nonlinear inverse problem described in Section II-A in an optimal fashion. The image s and noise n are assumed to be realizations of random vectors with pdfs p_S and p_N , respectively. The quantity of interest here is the posterior distribution $p_{S|Y}$ which provides a complete statistical characterization of the problem at hand. Using Bayes' rule, we get

$$p_{S|Y}(\mathbf{s}|\mathbf{y}) = \frac{p_{Y|S}(\mathbf{y}|\mathbf{s})p_{S}(\mathbf{s})}{\int_{\mathbb{R}^{K}} p_{Y|S}(\mathbf{y}|\mathbf{s})p_{S}(\mathbf{s}) \,d\mathbf{s}},$$
(13)

where $p_{Y|S}$ (a.k.a. the likelihood function) is the conditional distribution of the measurements given the image. In this section, we first characterize the likelihood function $p_{Y|S}$ which depends on the chosen noise model. We then discuss the prior distribution p_S , which in our framework is defined using a deep generative model. Finally, we detail a MCMC scheme to generate samples from the posterior distribution $p_{S|Y}$. This allows us to perform inference by computing point-estimates and the uncertainties associated with them.

A. Likelihood Function

The likelihood function $p_{Y|S}$ is determined by the statistical model for the measurement noise. For the additive noise in (4), it is given by

$$p_{Y|S}(\mathbf{y}|\mathbf{s}) = p_N(\mathbf{y} - \mathbf{H}\{\mathbf{s}\}). \tag{14}$$

In many imaging systems, there exist multiple sources of noise and so it is reasonable to assume a white Gaussian noise model

¹Since the total field $u(\mathbf{r})$ depends on the refractive index contrast $s(\mathbf{r})$, we also refer to its discretized version as $\mathbf{u}(\mathbf{s})$.

(AWGN) due to the central limit theorem. The likelihood function then is

$$p_{Y|S}(\mathbf{y}|\mathbf{s}) = \frac{1}{(2\pi\sigma^2)^{M/2}} \exp\left(-\frac{\|\mathbf{y} - \mathbf{H}\{\mathbf{s}\}\|_2^2}{2\sigma^2}\right), \quad (15)$$

where σ is the standard deviation of the Gaussian noise.

B. Prior Distribution

The choice of the distribution p_S reflects our prior knowledge about the image of interest. This information is crucial for the resolution of the inverse problem, especially when it is illposed. In the classical Bayesian methods, p_S is usually chosen from a family of distributions with closed-form analytical expressions such that it fits the characteristics of the image and also allows for efficient inference. Popular examples include the Gaussian and Markovian models. Instead, in our framework, we propose to leverage the power of neural networks to define a data-driven prior distribution.

We assume that we have access to a dataset containing sample images from the true unknown probability distribution p_{image} of our image of interest. Here, the idea is to approximate p_{image} with p_S that is defined by a deep generative model. More specifically, we consider generative models consisting of a generator network $G: \mathbb{R}^d \to \mathbb{R}^K$ $(d \ll K)$ that maps a low-dimensional latent space to the high-dimensional image space. This network takes a vector $\mathbf{z} \in \mathbb{R}^d$, which is sampled from some distribution p_Z (typically a Gaussian or Uniform distribution), as input and yields a sample image $G(\mathbf{z})$ as the output. Thus, the generator network G and the distribution p_Z implicitly characterize p_S and provide us with a way to directly sample from it. If this model is properly trained, the resulting p_S is close to p_{image} and the generated images are statistically similar to the ones in the dataset.

In our experiments (see Section IV), we use the well-known Wasserstein GANs (WGANs) [80] for our data-driven prior. We provide a brief description of WGANs in Appendix A.

Augmented Deep Generative Priors: Training deep generative models such as GANs requires large amounts of data and is a challenging task in general. Over the past few years, there have been several proposals for improving their performance and this has led to the development of better training schemes and network architectures. Most existing works use normalized datasets, where each image has the same range of pixel values, for their models. However, this is not suitable if we wish to use such models as priors in quantitative imaging (e.g, ODT). In these modalities, it is important to recover the actual values of the object (image) as compared to only the contrast. Thus, we require our generative model to be able to output images with different ranges of pixel values.

While performing our experiments, we observed that training high-quality WGANs on unnormalized datasets was non-trivial. We propose a simple effective work around, which simplifies the training and allows us to build models that generate images with different ranges. We define an augmented generative model $G_h: \mathbb{R}^{d+1} \to \mathbb{R}^K$ $(d \ll K)$ that consists of a (standard) generative network $G: \mathbb{R}^d \to \mathbb{R}^K$ trained on a

normalized dataset and a deterministic function $h: \mathbb{R} \to \mathbb{R}$. Here, the latent vector $\mathbf{z} = (\mathbf{z}_1, z_2) \in \mathbb{R}^{d+1}$ has two independent components $\mathbf{z}_1 \in \mathbb{R}^d$ and $z_2 \in \mathbb{R}$ that are sampled from p_{Z_1} and p_{Z_2} respectively, and the output image is given by $G_h(\mathbf{z}) = h(z_2)G(\mathbf{z}_1)$. For a generated image $G_h(\mathbf{z}) \in \mathbb{R}^K$, the term $G(\mathbf{z}_1) \in \mathbb{R}^K$ represents its details or contrast, and the term $h(z_2)$ represents its scaling factor. Since G is now required to only produce images with the same range, we can rely on existing GANs to obtain high-quality models. Moreoever, the distribution of the scaling factor can be easily controlled by carefully choosing the distribution p_{Z_2} and the function h.

C. Sampling from the Posterior Distribution

Now that we have described the likelihood function $p_{Y|S}$ and the prior distribution p_S , we look at the problem of drawing samples from the posterior distribution $p_{S|Y}$. Since our prior distribution p_S is defined by a pre-trained augmented deep generative model $G_h: \mathbb{R}^{d+1} \to \mathbb{R}^K: \mathbf{z} \mapsto G_h(\mathbf{z})$ with $p_Z(\mathbf{z}) = p_{Z_1}(\mathbf{z}_1)p_{Z_2}(z_2)$ for any $\mathbf{z} = (\mathbf{z}_1, z_2) \in \mathbb{R}^{d+1}$, we can focus on the posterior distribution $p_{Z|Y}$ of the latent vector instead. More specifically, if we generate a sample $\overline{\mathbf{z}}$ from $p_{Z|Y}$, then the image $\overline{\mathbf{s}} = G_h(\overline{\mathbf{z}})$ is a sample from $p_{S|Y}$.

In this work, we use the Metropolis-adjusted Langevin algorithm (MALA) [62], [63], which is a Markov Chain Monte Carlo (MCMC) method, to sample from $p_{Z\mid Y}$. The general idea in MCMC methods is to design a Markov chain whose stationary (or invariant) distribution is the target distribution that we want to sample from. If the chain is run for a sufficently long time, the generated samples (after the chain has converged) are indeed samples from the target distribution. The Markov property of the chain implies that each random sample only depends on the previous one.

Given a sample $\overline{\mathbf{z}}_t$, MALA generates the next one $\overline{\mathbf{z}}_{t+1}$ with the help of two steps. First, we construct a proposal $\widetilde{\mathbf{z}}_{t+1}$ for the new sample, which is given by

$$\widetilde{\mathbf{z}}_{t+1} = \overline{\mathbf{z}}_t + \tau \nabla_{\mathbf{z}} \log p_{Z|Y}(\overline{\mathbf{z}}_t|\mathbf{y}) + \sqrt{2\tau} \zeta,$$
 (16)

where ζ is drawn from the standard multivariate Gaussian distribution and $\tau > 0$ is a fixed step-size. In the second step, the proposal $\tilde{\mathbf{z}}_{t+1}$ is either accepted or rejected, with the acceptance probability being

$$\alpha = \min \left\{ 1, \frac{p_{Z|Y}(\widetilde{\mathbf{z}}_{t+1}|\mathbf{y})q_{\mathbf{y}}(\overline{\mathbf{z}}_{t}|\widetilde{\mathbf{z}}_{t+1})}{p_{Z|Y}(\overline{\mathbf{z}}_{t}|\mathbf{y})q_{\mathbf{y}}(\widetilde{\mathbf{z}}_{t+1}|\overline{\mathbf{z}}_{t})} \right\}, \tag{17}$$

where $q_{\mathbf{y}}(\overline{\mathbf{z}}|\widetilde{\mathbf{z}}) = \exp\left(-\frac{1}{4\tau}\|\overline{\mathbf{z}} - \widetilde{\mathbf{z}} - \tau \nabla_{\mathbf{z}} \log p_{Z|Y}(\widetilde{\mathbf{z}}|\mathbf{y})\|_2^2\right)$. If the proposal is accepted, we get our new sample $\overline{\mathbf{z}}_{t+1} = \widetilde{\mathbf{z}}_{t+1}$; otherwise we repeat the described two-step process. The stepsize τ is generally chosen to obtain a reasonable acceptance rate for the algorithm. One advantage of MALA is that it uses the gradient of the (log) target distribution to construct more probable proposals and so it is possible to achieve higher acceptance rates compared to other MCMC methods such as the Metropolis-Hastings algorithm [81].

The major computational bottleneck in MALA is the computation of the gradient term $\nabla_{\mathbf{z}} \log p_{Z|Y}$. If we assume an additive white Gaussian noise model with variance σ^2 and

that p_Z is the standard mutivariate Gaussian distribution, then $p_{Z|Y}$ can be written as

$$p_{Z|Y}(\mathbf{z}|\mathbf{y}) = \frac{1}{C} \exp\left(-\frac{\|\mathbf{y} - \mathbf{H}\{G_h(\mathbf{z})\}\|_2^2}{2\sigma^2} - \frac{\|\mathbf{z}\|_2^2}{2}\right), (18)$$

where C is the constant normalizing factor. In this case, the gradient term is

$$\nabla_{\mathbf{z}} \log p_{Z|Y}(\mathbf{z}|\mathbf{y}) = -\frac{\mathbf{J}_{G_h}^{H}(\mathbf{z})\mathbf{J}_{\mathbf{H}}^{H}(\mathbf{z})(\mathbf{y} - \mathbf{H}\{G_h(\mathbf{z})\})}{\sigma^2} - \mathbf{z}.$$
(19)

Since G_h is a neural network and **H** has a neural-network-like structure, we then compute this quantity efficiently using error backpropagation algorithms.

Once we obtain the samples $\{\overline{\mathbf{z}}_t\}_{t=1}^T$ from $p_{Z|Y}$, we transform them to get samples $\{G_h(\overline{\mathbf{z}}_t)\}_{t=1}^T$ from $p_{S|Y}$ and then use them to perform inference. Specifically, we can then approximate any integral of the form $\int_{\mathbb{R}^K} f(\mathbf{s}) p_{S|Y}(\mathbf{s}|\mathbf{y}) \, \mathrm{d}\mathbf{s}$, where $f: \mathbb{R}^K \to \mathbb{R}$ is a real-valued function, by its empirical estimate $E_T(f) = \frac{1}{T} \sum_{t=1}^T f(G_h(\overline{\mathbf{z}}_t))$. Although the generated samples are not independent due to the Markov property of the sequence, the Markov Chain Central Limit Theorem [82] ensures that $E_T(f)$ concentrates around the true value of the integral.

IV. EXPERIMENTAL RESULTS

In this section, we show the benefits of our neural-networkbased Bayesian reconstruction framework by applying it to phase retrieval and optical diffraction tomography problems.

A. Augmented WGANs

In our first experiment, we highlight the importance of the proposed augmented generative models. We consider the task of training WGAN models on datasets consisting of 128×128 images, where each image contains a constant-valued disc and its background pixels are zero-valued. The coordinates (x,y) of the center of the disc, its radius r (in pixels) and its constant value v follow the uniform distributions $U_{(10,115)}$, $U_{[4,25]}$ and $U_{(0,0.2]}$ respectively. The aforementioned parameters implicitly define the probability distribution $p_{\rm data}$ that we wish to approximate using WGANs.

We qualitatively compare the performance of two models. The first model is a WGAN trained on 50,000 images sampled from $p_{\rm data}$. In this case, the distribution p_Z for the latent variable is chosen to be the standard multivariate Gaussian distribution. The second model is an augmented WGAN, where the WGAN component is trained on a normalized dataset with 50,000 images. Thus, we first sample 50,000 images from $p_{\rm data}$ and we then normalize each of them such that the value of the disc is one. The distributions p_{Z_1} and p_{Z_2} are chosen to be standard Gaussian distributions as well, and the function h is

$$h(x) = \frac{0.2}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt.$$
 (20)

This choice of h and p_{Z_2} ensures that the scaling factor of the augmented WGAN follows the uniform distribution $U_{(0,0.2]}$.

The WGANs are trained for 2000 epochs using RMSProp optimizers with a learning rate of 5×10^{-5} and a batch size of 64. The parameters $\lambda_{\rm gp}$ and $n_{\rm critic}$ (refer to Appendix A) are set as 10 and 5, respectively. In Figure 4, we present typical samples generated by the two models. We see that the WGAN struggles to obtain piecewise constant discs. By contrast, the augmented WGAN consistently generates samples close to the target distribution.

B. Phase Retrieval

Next, we look at the phase retrieval problem. The ground-truth images for this set of experiments are taken from the MNIST [83] testing dataset which contains 28×28 images of handwritten digits. The chosen images are normalized to have values in the range [0,1], and then they are scaled by a factor randomly sampled from the uniform distribution $U_{(0,0.2]}$. The measurements $\mathbf{y} \in \mathbb{C}^M$ are simulated according to (6), where \mathbf{A} is a fixed random matrix with i.i.d. entries from a Gaussian distribution. This setup has been studied from a theoretical point of view in the literature and also corresponds to certain practical applications such as imaging in complex media.

We use an augmented model G_h to define the prior in our Bayesian framework. The WGAN component is trained on the MNIST training dataset which contains 50,000 images. The distributions p_{Z_1} and p_{Z_2} are Gaussian distributions and the function h is

$$h(x) = \frac{0.75}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt.$$
 (21)

The WGAN is trained for 500 epochs using ADAM optimizers with a learning rate of 2×10^{-4} and a batch size of 64. The parameters $\lambda_{\rm gp}$ and $n_{\rm critic}$ are set as 10 and 5, respectively.

As discussed in Section III-C, we draw samples from the posterior distribution using MALA. The step-size τ is set to 10^{-5} . We discard the first 100,000 samples in order to allow the Markov chain to converge. After this burn-in period, we collect the next 100,000 samples for performing inference. We compute the posterior mean which corresponds to the minimum mean-square error estimate. Further, to quantify the uncertainty associated with our estimation, we also compute the pixelwise variance map with the help of the samples from the posterior distribution.

Our results for M/K=0.5 and $\sigma^2=1$ are shown in Figure 5.

C. Optical Diffraction Tomography

For our ODT experiments, the test images are samples from the dataset described in Section IV-A. We simulate the ODT measurements by using BPM (Section II-C). We set the sampling steps $\delta_x, \delta_y = 0.1\,\mu\text{m}$, the medium RI $n_b = 1.52$, and the wavelength $\lambda = 0.406\,\mu\text{m}$. The RI of the sample is set to 1.62. We use Q = 15 incident tilted plane waves with angles that cover the range $\left[\frac{-\pi}{12}, \frac{\pi}{12}\right]$ and add a 20 dB Gaussian noise to the simulated total fields. The low number of measurements and the limited range of illumination angles yields a challenging reconstruction task. We reconstruct the RI

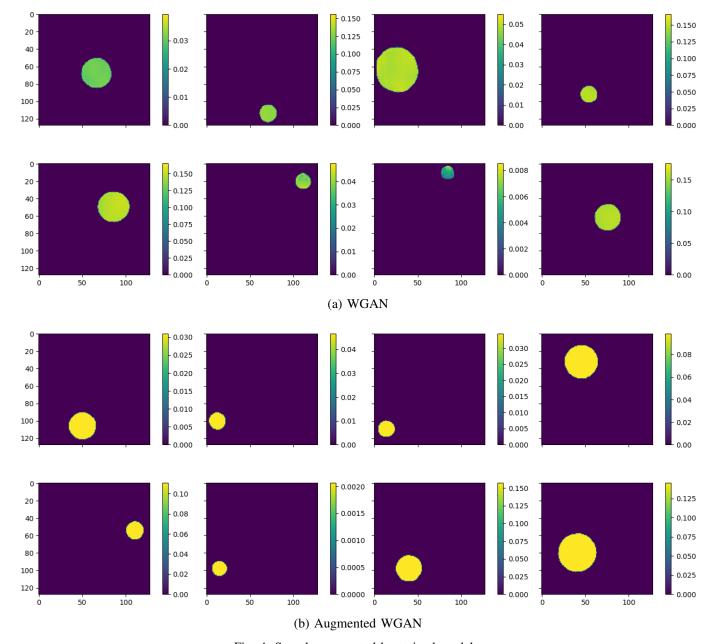


Fig. 4: Samples generated by trained models.

sample with two approaches: BPM with TV and BPM with the augmented WGAN prior from Section IV-A.

The regularization parameter for the TV reconstruction is set via a grid search. For MALA, the step-size τ is set to 10^{-6} . We discard the first 200,000 samples in order to allow the Markov chain to converge. After this burn-in period, we collect the next 100,000 samples for performing inference. We display the RI reconstructions in Figure 6. For our method, we show the posterior mean and pixelwise standard deviation map. We see that the proposed framework outperforms the the TV approach.

APPENDIX A WASSERSTEIN GENERATIVE ADVERSARIAL NETWORKS (WGANS)

Classical GANs [51] are known to suffer from issues such as the instability of the training process [84], [85], vanishing gradients and mode collapse. The framework of Wasserstein GANs [80] is an alternative that solves these problems.

Let \mathcal{D} be a dataset consisting of samples drawn from a probability distribution p_r . The goal is to build a model using \mathcal{D} that can generate samples which follow a distribution that closely approximates p_r . A WGAN consists of a generator network $G_{\theta}: \mathbb{R}^d \to \mathbb{R}^K$ $(d \ll K)$, where $\theta \in \mathbb{R}^{d_1}$ denotes its trainable parameters. It takes an input vector $\mathbf{z} \in \mathbb{R}^d$, which is sampled from a fixed distribution p_Z , and outputs $G_{\theta}(\mathbf{z}) \in \mathbb{R}^K$. The samples generated by this model follow

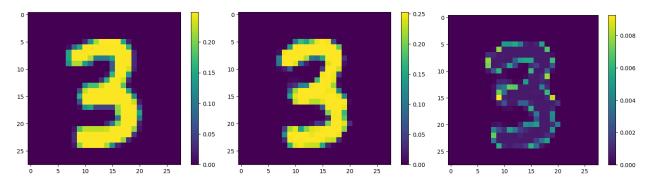


Fig. 5: From left to right: ground truth, posterior mean (SNR = 14.83 dB) and pixelwise standard deviation map.

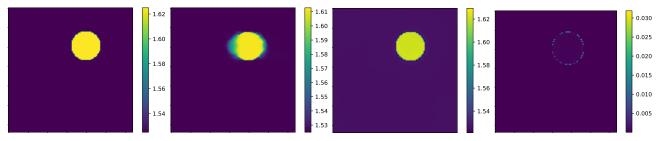


Fig. 6: RI reconstructions. From left to right: ground truth, reconstruction using BPM with TV (47.98 dB), posterior mean (57.82 dB) and pixelwise standard deviation map.

some distribution p_{θ} that is characterized by G_{θ} and p_Z . Thus, the parameters θ need to be chosen such that p_{θ} approximates p_r well.

In the WGAN framework, the generator is trained to minimize the Wasserstein-1 (or Earth-Mover) distance between p_r and p_{θ} , which is given by

$$W(p_{\mathbf{r}}, p_{\theta}) = \inf_{\gamma \in \pi(p_{\mathbf{r}}, p_{\theta})} \mathbb{E}_{(\mathbf{u}, \mathbf{v}) \sim \gamma} [\|\mathbf{u} - \mathbf{v}\|].$$
 (22)

Here, $\pi(p_r, p_{\theta})$ is the collection of all joint distributions with marginals p_r and p_{θ} respectively. The Kantorovich-Rubinstein duality theorem [86] states that (22) can be written as

$$W(p_{\mathbf{r}}, p_{\theta}) = \sup_{f \in \mathcal{X}} \mathbb{E}_{\mathbf{u} \sim p_{\mathbf{r}}}[f(\mathbf{u})] - \mathbb{E}_{\mathbf{v} \sim p_{\theta}}[f(\mathbf{v})], \quad (23)$$

where $\mathcal{X} = \{f : \mathbb{R}^K \to \mathbb{R} \mid f \text{ is 1-Lipschitz}\}$. The space \mathcal{X} is then replaced by a family of 1-Lipschitz functions represented by a critic neural network $D_{\phi} : \mathbb{R}^K \to \mathbb{R}$ with appropriately constrained parameters $\phi \in \mathbb{R}^{d_2}$. This leads to the following minimax problem for training the model:

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^{d_1}} \max_{\boldsymbol{\phi} \in \mathcal{Y}} \mathbb{E}_{\mathbf{u} \sim p_{\mathsf{r}}}[D_{\boldsymbol{\phi}}(\mathbf{u})] - \mathbb{E}_{\mathbf{v} \sim p_{\boldsymbol{\theta}}}[D_{\boldsymbol{\phi}}(\mathbf{v})], \quad (24)$$

where $\mathcal{Y}=\{\phi\in\mathbb{R}^{d_2}\mid \mathrm{D}_{\phi} \text{ is 1-Lipschitz}\}$. In [80], the authors enforce the 1-Lipschitz condition on D_{ϕ} by clipping its weights during training. However, as shown in [87], this approach can cause difficulties in the optimization process. Instead, the 1-Lipschitz constraint can be enforced by adding a gradient penalty to the cost function in (24). The regularized

minimax problem is

$$\min_{\boldsymbol{\theta} \in \mathbb{R}^{d_1}} \max_{\boldsymbol{\phi} \in \mathbb{R}^{d_2}} \left(\mathbb{E}_{\mathbf{u} \sim p_r}[D_{\boldsymbol{\phi}}(\mathbf{u})] - \mathbb{E}_{\mathbf{v} \sim p_{\boldsymbol{\theta}}}[D_{\boldsymbol{\phi}}(\mathbf{v})] + \lambda_{gp} \mathbb{E}_{\mathbf{w} \sim p_{int}}[(\|\nabla_{\mathbf{w}}D_{\boldsymbol{\phi}}(\mathbf{w})\| - 1)^2] \right), \quad (25)$$

where a point $\mathbf{w} \sim p_{\text{int}}$ is obtained by sampling unformly along straight lines between points drawn from p_{r} and p_{θ} , and $\lambda_{\text{gp}} > 0$ is a hyperparameter.

In practice, Problem (25) is solved using mini-batch stochastic gradient algorithms in an alternating manner. During each iteration for the critic, we collect a batch of samples $\{\mathbf{x}_n\}_{n=1}^{N_c}$ from the dataset \mathcal{D} . We sample vectors $\{\mathbf{z}_n\}_{n=1}^{N_c}$ from p_Z and a sequence of numbers $\{\alpha_n\}_{n=1}^{N_c}$ from the uniform distribution $U_{[0,1]}$, and we construct $\mathbf{w}_n = \alpha_n \mathbf{x}_n + (1-\alpha_n) \mathbf{G}_{\boldsymbol{\theta}}(\mathbf{z}_n)$. The critic parameters are then updated by ascending along the gradient given by

$$\frac{1}{N_c} \nabla_{\phi} \left(\sum_{n=1}^{N_c} \mathcal{D}_{\phi}(\mathbf{x}_n) - \mathcal{D}_{\phi}(\mathcal{G}_{\theta}(\mathbf{z}_n)) + \lambda_{gp} (\|\nabla_{\mathbf{w}_n} \mathcal{D}_{\phi}(\mathbf{w}_n)\| - 1)^2 \right).$$
(26)

During each iteration for the generator, we sample latent vectors $\{\mathbf{z}_n\}_{n=1}^{N_g}$ from p_Z . The generator parameters are then updated by descending along the gradient given by

$$\frac{1}{N_g} \nabla_{\boldsymbol{\theta}} \left(\sum_{n=1}^{N_g} -D_{\boldsymbol{\phi}}(G_{\boldsymbol{\theta}}(\mathbf{z}_n)) \right). \tag{27}$$

Typically, for every generator iteration, the critic is trained for n_{critic} iterations.

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