Abstract

We develop a novel method for carrying out model selection for Bayesian autoencoders (BAEs) by means of prior hyper-parameter optimization. Inspired by the common practice of type-II maximum likelihood optimization and its equivalence to Kullback-Leibler divergence minimization, we propose to optimize the distributional sliced-Wasserstein distance (DSWD) between the output of the autoencoder and the empirical data distribution. The advantages of this formulation are that we can estimate the DSWD based on samples and handle high-dimensional problems. We carry out posterior estimation of the BAE parameters via stochastic gradient Hamiltonian Monte Carlo and turn our BAE into a generative model by fitting a flexible Dirichlet mixture model in the latent space. Consequently, we obtain a powerful alternative to variational autoencoders, which are the preferred choice in modern applications of autoencoders for representation learning with uncertainty. We evaluate our approach qualitatively and quantitatively using a vast experimental campaign on a number of unsupervised learning tasks and show that, in small-data regimes where priors matter, our approach provides state-of-the-art results, outperforming multiple competitive baselines.

1 Introduction

The problem of learning useful representations of data that facilitate the solution of downstream tasks such as clustering, generative modeling and classification, is at the crux of the success of many machine learning applications [see, e.g., 5, and references therein]. From a plethora of potential solutions to this problem, unsupervised approaches based on autoencoders [13] are particularly appealing as, by definition, they do not require label information and have proved effective in tasks such as dimensionality reduction and information retrieval [27].

Autoencoders are neural network models composed of two parts, usually referred to as the encoder and the decoder. The encoder maps each input $x_i$ to a set of lower-dimensional latent variables $z_i$. The decoder maps the latent variables $z_i$ back to the observations $x_i$. The bottleneck introduced by the low-dimensional latent space is what characterizes the compression and representation learning capabilities of autoencoders. It is not surprising that these models have connections with principal component analysis [3], factor analysis and density networks [41], and latent variable models [35].

In applications where quantification of uncertainty is a primary requirement or where data is scarce, it is important to carry out a Bayesian treatment of these models by specifying a prior distribution over their parameters, i.e., the weights of the encoder/decoder. However, estimating the posterior distribution over the parameters of these models, which we refer to as Bayesian autoencoders (BAEs),
is generally intractable and requires approximations. Furthermore, the need to specify priors for a large number of parameters, coupled with the fact that autoencoders are not generative models, has motivated the development of Variational Autoencoders (VAEs) as an alternative that can overcome these limitations [32]. Indeed, VAEs have found tremendous success and have become one of the preferred methods in modern machine-learning applications [see, e.g., 33, and references therein].

To recap, three potential limitations of BAEs hinder their widespread applicability in order to achieve a similar or superior adoption to their variational counterpart: (i) lack of generative modeling capabilities; (ii) intractability of inference and (iii) difficulty of setting sensible priors over their parameters. In this work we revisit BAEs and deal with these limitations in a principled way. In particular, we address the first limitation in (i) by employing density estimation in the latent space. Furthermore, we deal with the second limitation in (ii) by exploiting recent advances in Markov chain Monte Carlo (MCMC) and, in particular, stochastic gradient Hamiltonian Monte Carlo (SGHMC) [11]. Finally, we believe that the third limitation (iii), which we refer to as the difficulty of carrying out \textit{model selection}, requires a more detailed treatment because choosing sensible priors for Bayesian neural networks is an extremely difficult problem, and this is the main focus of this work.

**Contributions.** Specifically, in this paper we provide a novel, practical, and elegant way of performing model selection for BAEs, which allows us to revisit these models for applications where VAEs are currently the primary choice. We start by considering the common practice of estimating prior (hyper-)parameters via type-II maximum likelihood, which is equivalent to minimizing the Kullback-Leibler divergence (KL) between the distribution induced by the BAE and the data generating distribution. Because of the intractability of this objective and the difficulty to estimate it through samples, we resort to an alternative formulation where we replace the KL with the distributional sliced-Wasserstein distance (DSWD) between these two distributions. The advantages of this formulation are that we can estimate the DSWD based on samples and, thanks to the slicing, we can handle large dimensional problems. Once BAE hyper-parameters are optimized, we estimate the posterior distribution over the BAE parameters via SGHMC [11], which is a powerful sampler that operates on mini-batches and has proven effective for Bayesian deep/convolutional networks [29, 60, 68]. Furthermore, we turn our BAE into a generative model by fitting a flexible mixture model in the latent space, namely the Dirichlet Process Mixture Model (DPMM). We evaluate our approach qualitatively and quantitatively using a vast experimental campaign on a number of unsupervised learning tasks, with particular emphasis on the challenging task of generative modeling when the number of observations is small.

### 1.1 Related work

VAEs provide a theoretically-grounded and popular framework for representation learning and deep generative modeling. However, training VAEs poses considerable practical and theoretical challenges yet to be solved. In practice, the learned aggregated posterior distribution of the encoder rarely matches the latent prior, and this hurts the quality of generated samples. Several methods have been proposed to deal with this problem by using a more expressive form of priors on the latent space [4, 12, 48, 59]. Similar to our work, there is a line of research that employs a form of ex-post density estimation on the learned latent space [8, 14, 19]. Wasserstein Autoencoders (WAEs) [58] impose a new form of regularization on latent space by reformulating the objective function as an optimal transport (OT) problem. There have been previous attempts to apply the Bayesian approach to VAEs. For example, [16] treats the parameters of VAE’s encoder and decoder in a Bayesian manner to deal with out-of-distribution samples. Most of these works focus on imposing prior or regularization on the latent or weight space of autoencoders. In this work, we take a different route, as we aim to impose prior knowledge directly on the output space. Indeed, our work is motivated by recent attempts to rethink prior specification for Bayesian neural networks (BNNs). It is extremely difficult to choose a sensible prior on the parameters of BNNs [see, e.g., 46, and references therein] because their effect on the distribution of the induced functions is difficult to characterize. Thus, recent attempts in the literature have turned their attention towards defining priors in the space of functions [22, 47, 57, 65]. Closest to our work is that of [60], which matches the functional prior induced by BNNs to Gaussian Process (GP) priors by means of the Kantorovich-Rubinstein dual form of the Wasserstein distance. Different from this line of works, we consider a general framework to impose a functional prior for BNNs in an unsupervised learning setting.
2 Preliminaries on Bayesian Autoencoders

An autoencoder (AE) is a neural network parameterized by a set of parameters \( w \), which transforms an unlabelled dataset, \( x \overset{\text{def}}{=} \{ x_n \}_{n=1}^N \), into a set of reconstructions \( \hat{x} \overset{\text{def}}{=} \{ \hat{x}_n \}_{n=1}^N \), with \( x_n, \hat{x}_n \in \mathbb{R}^D \). An AE is composed of two components: (1) an encoder \( f_{\text{enc}} \) which maps an input sample \( x_n \) to a latent code \( z_n \in \mathbb{R}^K \), \( K \ll D \); and (2) a decoder \( f_{\text{dec}} \) which maps the latent code to a reconstructed datapoint \( \hat{x}_n \). In short, \( \hat{x} = f(x; w) = (f_{\text{dec}} \circ f_{\text{enc}})(x) \), where we denote \( w := \{ w_{\text{enc}}, w_{\text{dec}} \} \) the union of parameters of the encoder and decoder. The Bayesian treatment of AEs dictates that a prior distribution \( p(w) \) is placed over all parameters of \( f_{\text{enc}} \) and \( f_{\text{dec}} \), and that this prior knowledge is transformed into a posterior distribution by means of Bayes’ theorem,

\[
p(w | x) = \frac{p(x | w)p(w)}{p(x)},
\]

where \( p(x | w) \) is the conditional likelihood that factorizes as \( p(x | w) = \prod_{n=1}^N p(x_n | w) \). Note that each conditional likelihood term is determined by the model architecture, the choice of \( w \), and the input \( x_n \), but in order to keep the notation uncluttered, we write them simply as \( p(x_n | w) \).

Likelihood model. In the Bayesian scheme, the prior and likelihood are both modeling choices. Before giving an in-depth treatment on priors for BAES in the next section, we briefly discuss the likelihood, which can be chosen according to the type of data. In our experiments, we mainly investigate image datasets, where pixel values are normalized in the \([0, 1]\) range. Therefore, we rely on the continuous Bernoulli distribution [39]:

\[
p(x_n | w) = \prod_{i=1}^D K(\lambda_i) \lambda_i^{x_{n,i}} (1 - \lambda_i)^{1-x_{n,i}} := p(x_n | \hat{x}_n),
\]

where \( K(\lambda_i) \) is a properly defined normalization constant [39] and \( \lambda_i = f_i(x_n; w) = \hat{x}_{n,i} \in [0, 1] \) is the \( i \)-th output from the BAE given the input \( x_n \). We note that, as \( \hat{x}_n \) depends deterministically on \( w \), we will use the above expression to refer to both \( p(x_n | w) \) and \( p(x_n | \hat{x}_n) \), where the latter term will be of crucial importance when we define the functional prior induced over the reconstruction \( \hat{x} \).

Inference. Although the posterior of BAES is analytically intractable, it can be approximated by variational methods or using MCMC sampling. Within the large family of approximate Bayesian inference schemes, SGHMC [11] allows us to sample from the true posterior by efficiently simulating a Hamiltonian system [49]. Differently from more traditional methods, SGHMC can scale up to large datasets by relying on noisy but unbiased estimates of the potential energy function \( U(w) = -\sum_{n=1}^N \log p(x_n | w) - \log p(w) \). These can be computed by considering a mini-batch of size \( M \) of the data and approximating \( \sum_{n=1}^N \log p(x_n | w) \approx \frac{N}{M} \sum_{j \in I_M} \log p(x_j | w) \), where \( I_M \) is a set of \( M \) random indices. More details on SGHMC can be found in the Appendix.

Pathologies of standard priors. The choice of the prior is important for the Bayesian treatment of any model as it characterizes the hypothesis space [42, 45]. Specifically for BAES, one should note that placing a prior on the parameters of the encoder and decoder has an implicit effect on the prior over the network output (i.e. the reconstruction). In addition, the highly nonlinear nature of these models implies that interpreting the effect of the architecture is theoretically intractable and practically challenging. Several works argue that a vague prior such as \( \mathcal{N}(0, 1) \) is good enough for some tasks and models, like classification with convolutional neural networks (CNNs) [64].

However, for BAES this is not enough, as illustrated in Fig. 1. The realizations obtained by sampling weights/biases from a \( \mathcal{N}(0, 1) \) prior indicate that this choice provides poor inductive bias. Meanwhile, by encoding better beliefs via an optimized prior, which is the focus of the next section, the samples

| Input | Output with \( \mathcal{N}(0, 1) \) Prior | Output with Optimized Prior |
|-------|--------------------------------|-----------------------------|
| MNIST | ![MNIST](image1.png) | ![MNIST](image2.png) |
| OOD   | ![OOD](image3.png) | ![OOD](image4.png) |
| CELEBA| ![CELEBA](image5.png) | ![CELEBA](image6.png) |
| OOD   | ![OOD](image7.png) | ![OOD](image8.png) |

Figure 1: Realizations sampled from different priors given an input image. OOD stands for out-of-distribution.
can capture main characteristics intrinsic to the data, even when the model is fed with out-of-distribution inputs.

3 Model Selection for Bayesian Autoencoders via Prior Optimization

One of the main advantages of the Bayesian paradigm is that we can incorporate prior knowledge into the model in a principled way. Let us assume a prior distribution \( p_\psi(w) \) on the parameters of the AE network, where now we are explicit on the set of (hyper-)parameters that determine the prior, i.e., \( \psi \). Specifying this prior for the BAE is not straightforward due to the complex nonlinear forms of \( f_{\text{enc}} \) and \( f_{\text{dec}} \), which induce a non-trivial effect on the output (functional) prior:

\[
p_\psi(\hat{x}) = \int f(x; w)p_\psi(w)dw,
\]

where \( \hat{x} = f(x; w) \) is the functional output of the BAE. Although \( p_\psi(\hat{x}) \) cannot be evaluated analytically, it is possible to draw samples from it.

Prior parameterization. The only two requirements needed to design a parameterization for the prior are: to be able to (1) draw samples from it and (2) to compute its log-density at any point. The latter is required by many inference algorithms such as SGHMC. We consider a fully-factorized Gaussian prior over weights and biases at layer \( l \):

\[
p(w_l) = \mathcal{N}(w_l; \mu_{w_l}, \sigma_{w_l}^2), \quad p(b_l) = \mathcal{N}(b_l; \mu_{b_l}, \sigma_{b_l}^2),
\]

Notice that, as we shall see in § 3.2 and § 3.3, in order to estimate our prior hyper-parameters, we will need gradient back-propagation through the stochastic variables \( w_l \) and \( b_l \). Thus, we treat these parameters in a deterministic manner by means of the reparameterization trick [32, 55].

3.1 Another route for Bayesian Occam’s razor

A common way to estimate hyper-parameters (i.e., prior parameters \( \psi \)) is to rely on the Bayesian Occam’s razor (a.k.a. empirical Bayes), which dictates that the marginal likelihood \( p_\psi(x) \) should be optimized with respect to \( \psi \). There are countless examples where such simple procedure succeeds in practice [see, e.g., 54].

The marginal likelihood is obtained by marginalizing out the outputs \( \hat{x} \) and the model parameters \( w \),

\[
p_\psi(x) = \int p(x | \hat{x})p_\psi(\hat{x})d\hat{x},
\]

where \( p(x | \hat{x}) \) and \( p_\psi(\hat{x}) \) are given by Eq. 2 and Eq. 3, respectively. Unfortunately, in our context it is impossible to carry out this optimization due to the intractability of Eq. 5.

Classic results in the statistics literature draw parallels between maximum likelihood estimation (MLE) and KL minimization [2],

\[
\arg \max_\psi \int \pi(x) \log p_\psi(x) dx = \arg \min_\psi \int \pi(x) \log \frac{\pi(x)}{p_\psi(x)} dx,
\]

where \( \pi(x) \) is the true data distribution. This equivalence provides us with an interesting insight on an alternative view of marginal likelihood optimization as minimization of the divergence between the true data distribution and the marginal \( p_\psi(x) \).

This alternative view still does not help us in obtaining a viable optimization strategy, even if we use \( x \) to estimate an empirical \( \hat{\pi}(x) \); the empirical evaluation and optimization of \( \psi \) is indeed a well-known challenging problem [18], although this is possible (for the KL or any other \( f \)-divergence), for example, by leveraging results from convex analysis such as in the convex minimization framework of [51]. However, we can now attempt to replace the intractable KL divergence with another divergence to recover tractability. Inspired by recent works on deriving sensible priors for Bayesian neural networks [60], we employ the Wasserstein distance, which, as we will see later, can be estimated efficiently using samples only, even for high-dimensional distributions.

To summarize: (1) we would like to do prior selection by carrying out type-II MLE; (2) the MLE objective is analytically intractable but the connection with KL minimization allows us to (3) swap the divergence with the Wasserstein distance, yielding a practical framework for choosing priors.
3.2 Matching the marginal distribution to the data distribution via Wasserstein distance minimization

Given the two probability measures \( \pi \) and \( p_\psi \), both defined on \( \mathbb{R}^D \) for simplicity, the \( p \)-Wasserstein distance between \( \pi \) and \( p_\psi \) is given by

\[
W_p^p(\pi, p_\psi) = \inf_{\gamma \in \Gamma(\pi, p_\psi)} \int \| x - x' \|^p \gamma(x, x') \, dx \, dx',
\]

where \( \Gamma(\pi, p_\psi) \) is the set of all possible distributions \( \gamma(x, x') \) such that the marginals are \( \pi(x) \) and \( p_\psi(x') \) [62]. While usually analytically unavailable or computationally intractable, for \( D = 1 \) the distance has a simple closed form solution, that can be easily estimated using samples only [34].

The distributional sliced-Wasserstein distance (DSWD) takes advantage of this result by projecting the estimation of distances for high-dimensional distributions into simpler estimation of multiple distances in one dimension. The projection is done using the Radon transform, an operator that maps a generic density function \( \varphi \) defined in \( \mathbb{R}^D \) to the set of its integrals over hyperplanes in \( \mathbb{R}^D \),

\[
\mathcal{R}\varphi(t, \theta) := \int \varphi(x) \delta(t - x^\top \theta) \, dx, \quad \forall t \in \mathbb{R}, \quad \forall \theta \in \mathbb{S}^{D-1},
\]

where \( \mathbb{S}^{D-1} \) is the unit sphere in \( \mathbb{R}^D \) and \( \delta(\cdot) \) is the Dirac delta [24]. Using the Radon transform, for a given direction (or slice) \( \theta \) we can project the two densities \( \pi \) and \( p_\psi \), into one dimension and we can solve the optimal transport problem in this projected space. Furthermore, to avoid unnecessary computations, instead of considering all possible directions in \( \mathbb{S}^{D-1} \), DSWD proposes to find the optimal probability measure of slices \( \sigma(\theta) \) on the unit sphere \( \mathbb{S}^{D-1} \),

\[
DSW_p^p(\pi, p_\psi) := \sup_{\sigma \in \mathcal{M}_C} \left( \mathbb{E}_{\sigma(\theta)} W_p^p(\mathcal{R}\pi(t, \theta), \mathcal{R}p_\psi(t, \theta)) \right)^{1/p},
\]

where, for \( C > 0 \), \( \mathcal{M}_C \) is the set of probability measures \( \sigma \) such that \( \mathbb{E}_{\sigma(\theta', \theta)} [\theta^\top \theta'] \leq C \) (a constraint that aims to avoid directions to lie in only one small area). The direct computation of \( DSW_p^p \) in Eq. 9 is still challenging but admits an equivalent dual form,

\[
\sup_{\mathcal{H}} \left\{ \left( \mathbb{E}_{\sigma(\theta)} W_p^p(\mathcal{R}\pi(t, h(\theta)), \mathcal{R}p_\psi(t, h(\theta))) \right)^{1/p} - \lambda C \mathbb{E}_{\sigma(\theta', \theta)} [h(\theta)^\top h(\theta')] \right\} + \lambda C C,
\]

where \( \sigma \) is a uniform distribution in \( \mathbb{S}^{D-1} \), \( \mathcal{H} \) is the set of functions \( h : \mathbb{S}^{D-1} \rightarrow \mathbb{S}^{D-1} \) and \( \lambda C \) is a regularization hyper-parameter. The formulation in Eq. 10 is obtained by employing the Lagrangian duality theorem and by reparameterizing \( \sigma(\theta) \) as push-forward transformation of a uniform measure in \( \mathbb{S}^{D-1} \) via \( h \). Now, by parameterizing \( h \) using a deep neural network with parameters \( \phi \), defined as \( h_\phi \), Eq. 10 becomes an optimization problem with respect to the network parameters. The final step is to approximate the analytically intractable expectations with Monte Carlo integration,

\[
\max_{\phi} \left\{ \left[ \frac{1}{K} \sum_{i=1}^K W_p^p(\mathcal{R}\pi(t, h_\phi(\theta_i)), \mathcal{R}p_\psi(t, h_\phi(\theta_i))) \right]^{1/p} - \frac{\lambda C}{K^2} \sum_{i,j=1}^K |h_\phi(\theta_i)^\top h_\phi(\theta_j)| \right\} + \lambda C C,
\]

with \( \theta_i \sim \tilde{\sigma}(\theta) \). Finally, we can use stochastic gradient methods to update \( \phi \) and then use the resulting optima for the estimation of the original distance. We encourage the reader to check the detailed explanation of this formulation, including its derivation and some practical considerations for implementation, available in the Appendix.

3.3 Summary

We aim at learning the prior on the BAE parameters by optimizing the marginal \( p_\psi(x) \) obtained after integrating out the weights from the joint \( p_\psi(x, w) \). The connection with empirical Bayes and KL minimization suggests that we can find the optimal \( \psi^* \) by minimizing the KL between the true data distribution \( \pi(x) \) and the marginal \( p_\psi(x) \). However, matching these two distributions is non-trivial due to their high dimensionality and the unavailability of their densities. To overcome this problem, we propose a sample-based approach using the distributional sliced-2-Wasserstein distance (Eq. 10) as objective:

\[
\psi^* = \arg \min_{\psi} \left[ DSW_2(p_\psi(x), \pi(x)) \right].
\]
This objective function is flexible and does not require the closed-form of either \( p_\psi(x) \) or \( \pi(x) \). The only requirement is that we can draw samples from these two distributions. Note that we can sample from \( p_\psi(x) \), by first computing \( \hat{x} \) after sampling from \( p_\psi(w) \) and then perturbing the generated \( \hat{x} \) by sampling from the likelihood \( p(x | \hat{x}) \). For the continuous Bernoulli likelihood this operation can be implemented by using the reparameterization form that allows to backpropagate gradients [39].

4 Experiments

Competing approaches. We compare our proposal with a wide selection of methods from the literature. For autoencoding methods, we choose the vanilla VAE [32], the \( \beta \)-VAE [26] and WAE (Wasserstein AE) [58]. In addition, we consider models with more complex encoders (VAE + Sylvester flows [61]), generators (2-stage VAE [14]), and priors (VAE + VampPrior [59]). For CELEBA we also include a comparison with Generative Adversarial Networks (GANs), with the vanilla setup of NS-GAN [21, 40] and the more recent DiffAugment-GAN [30, 69]. Finally, we also compare against BAE with the standard \( \mathcal{N}(0, 1) \) prior. Unless otherwise stated, all models—including ours—share the same latent dimensionality (\( K = 50 \)). We defer a more detailed description of these models and architectures to the Appendix.

Generative process. Differently from VAEs and other methods, deterministic and Bayesian AEs are not generative models. To generate new samples with BAEs we employ ex-post density estimation over the learned latent space, by fitting a density estimator \( p_\theta(z) \) to \( \{ z_i = \mathbb{E}_{p\left(w_{\text{enc}} | x\right)}[f_{\text{enc}}(x_i; w_{\text{enc}})] \} \). In this work, we employ a nonparametric model for density estimation based on Dirichlet Process Mixture Model (DPMM) [7], so that its complexity is automatically adapted to the data; see also [6] for alternative ways to turn AEs into generative models. After estimating \( p_\theta(z) \), a new sample can be generated by drawing \( z_{\text{new}} \) from \( p_\theta(z) \) and \( s_{\text{new}} = \mathbb{E}_{p\left(w_{\text{enc}} | x\right)}[f_{\text{dec}}(z_{\text{new}}; w_{\text{dec}})] \).

Evaluation metrics. To evaluate the reconstruction quality, we use the test log-likelihood (LL), which tells us how likely the test targets are generated by the corresponding model. The predictive log-likelihood is a proper scoring rule that depends on both the accuracy of predictions and their uncertainty [20]. To assess the quality of the generated images, instead, we employ the widely used Fréchet Inception Distance (FID) [25]. We note that, as GANS are not inherently equipped with an explicit likelihood model, we only report their FID scores. Finally, all our experiments and evaluations are repeated four times, with different random training splits.

4.1 Analysis of the effect of the prior

To demonstrate the effect of our model selection strategy, we consider scenarios in the small-data regime where the prior might not be necessarily tuned on the training set. In this way we are able to impose inductive bias beyond what is available in the training data. We investigate two cases:

- MNIST [36]: We use 100 examples of the 0 digits to tune the prior. The training set consists of examples of 1-9 digits, whereas the test set contains 10,000 instances of all digits. We aim to demonstrate the ability of our approach to incorporate prior knowledge about completely unseen data with different characteristics into the model.

- FREY-YALE [15]: We use 1,956 examples of FREY faces to optimize the prior. The training set and test set are comprised of YALE faces. We demonstrate the benefit of using a different dataset but from the same domain (e.g., face images) to specify the prior distribution.

Visual inspection. Fig. 2 shows some qualitative results (additional images are available in the Appendix), while Fig. 3 shows the convergence of the Wasserstein distance during prior optimization in our proposal. From a visual inspection we see that, on MNIST, by encoding knowledge about the “0” digit into the prior, the BAE can reconstruct this digit fairly well although we only use “1” to “9” digits for inference (differently from the BAE with standard prior). Similarly, on FREY-YALE, we see that by encoding knowledge from another dataset in the same domain, the optimized prior can impose a softer constraint compared to using directly this dataset for inference. In addition, if we use directly the union of FREY and YALE faces for training (methods denoted with a ⋄), VAE yields images that are similar to FREY instead of YALE faces, while generated images from BAE with \( \mathcal{N}(0, 1) \) prior are of lower quality. This again highlights the advantage of our approach to specifying an informative prior compared to using that data for training. Another important benefit of our Bayesian treatment of AEs is that we can quantify the uncertainty for both reconstructed and generated images. The last row of Fig. 2 illustrates the uncertainty estimate corresponding to the BAE with optimized prior on
MNIST and YALE datasets. Our model exhibits increased uncertainty for semantically and visually challenging pixels such as the left part of the second "0" digit image in the MNIST example. We also observe that the uncertainty is greater for generated images compared to reconstructed images as illustrated in the YALE example. This is reasonable because the reconstruction process is guided by the input data rather than synthesizing new data according to a random latent code.

**Visualization of inductive bias on MNIST.** To have an intuition of the inductive bias induced by the optimized prior, we visualize a low-dimensional projection of parameters sampled from the prior and the posterior [28]. As we see in Fig. 5, the hypothesis space induced by the $\mathcal{N}(0, 1)$ prior is huge, compared to where the true solution should lie. Effectively this is another visualization of the famous Bayesian Occam’s razor plot by David MacKay [43], where the model has very high complexity and poor inductive biases. On the other hand, by considering our proposal to do model selection, the hypothesis space of the optimized prior is reduced to regions close to the full posterior. Additional visualizations are available in the Appendix.

**Quantitative evaluation.** For a quantitative analysis we rely on Fig. 4, where we study the effect on the reconstruction quality of different training sizes (on the left) and different latent dimensions (on the right). Since we observed that the results of VAE variants are not significantly different, we only show the results for $\beta$-VAE and we leave the extended results to the Appendix. From this experiment we can draw important conclusions. The BAE with optimized priors clearly outperforms the competing methods (and the BAE with standard prior) in the inference task for all training sizes,
4.2 Reconstruction and generation of CELEBA

We now look at a more challenging benchmark, the CELEBA dataset [38]. For our proposal, we use 1000 examples that are randomly chosen from the original training set to learn the prior distribution. The test set consists of about 20,000 images. The goal of this experiment is to evaluate whether sacrificing part of the training data to specify a good prior is beneficial when compared to using that data for training the model. Fig. 6 shows qualitative results for the competing methods, their corresponding test LLs and FIDs for different training dataset sizes. In terms of test log-likelihoods (LLs) (Fig. 6, top right), we observe two clear patterns: (i) that BAE approaches perform considerably better than other methods and (ii) the VAE with Sylvester flows performs consistently poor across dataset sizes. This latter observation indicates that having a more expressive posterior for the encoder is not helpful when considering the small training sizes used in our experiments. More importantly, we see that the BAE using the optimized prior significantly outperforms other methods despite using less data for inference. These results largely agree with the quality of the reconstructions (first column of images in Fig. 6, left) in that BAE methods provide more visually appealing reconstructions when compared to other approaches.

We now evaluate the quality of the generated images (second column of images in Fig. 6, left) along with their FID scores [25]. Visually, it is clear that images generated from VAEs (standard, $\beta$, Sylvester and WAE) are very poor. This failure may originate from the fact that the aggregated posterior distribution of the encoder is not aligned with the prior on the latent space. This problem is more prominent in the case of small training data, where the encoder is not well-trained. The VampPrior tackles this problem by explicitly modeling the aggregated posterior, while 2-stage VAE uses another VAE to estimate the density of the learned latent space. By reducing the effect of the aggregated posterior mismatch, these strategies improve the quality of the generated images remarkably. These results are consistent with their corresponding FID scores (Fig. 6, bottom right) where we also see that BAE using the optimized prior consistently outperforms all variants of VAEs and NS-GAN. Finally, we see that DiffAugment-GAN, with the exception of using a training size of 500, yields better FID scores. However, this is not surprising as this model uses much more complex network architectures [30], combined with a powerful differentiable augmentation scheme. More importantly, it is clear that with few training samples our method generates more semantically meaningful images than all other approaches, including DiffAugment-GAN.
4.3 Prior adjustment versus posterior tempering

We have shown that the proposed framework for adjusting the prior is compatible with standard Bayesian practices, as it emulates type-II maximum likelihood. In other words, the distribution fitting that we induce by means of Wasserstein distance minimization relates to the marginal output of BAEs, very much in the same spirit of marginal likelihood maximization. The distribution is fit considering all possible functions, when marginalized through the likelihood, creating an implicit regularization effect. Our scheme does not give more weight to particular training instances, but it simply restricts the hypothesis space. This is unlike posterior tempering \cite{1, 28, 63, 66, 67}, which is commonly defined as $p_e(w \mid x) \propto p(x \mid w)^{1/\tau} p(w)$, where $\tau > 0$ is a temperature value. With $\tau < 1$, tempering is known to improve performance in the case of small training data and using miss-specified priors, but it corresponds to artificially sharpening the posterior by over-counting the data $\tau$ times.

To demonstrate the differences with our proposal, we setup a comparison on MNIST. In the empirical comparison of Fig. 7, we consider different temperatures and different sets of data points used to optimize the prior. As expected, the tempered posterior quickly collapses on the mode, while the posterior after our treatment retains a sufficiently constant variance, regardless of the number of data points used. It is also interesting to notice that with the $N(0, 1)$ prior, the best temperature is $\tau = 0.1$, while for our approach that optimizes the prior is $\tau = 1$, further confirming that the model now is well specified (Fig. 8).

![Performance at different temperatures $\tau$](image1)

**Figure 8:** Test performance for temperature scaling with different priors. The dotted lines indicate the best performance.

5 Conclusions

In this work, we have reconsidered the Bayesian treatment of autoencoders (AE) in light of recent advances in Bayesian neural networks. We have addressed the main challenge of BAEs, so that they can be rendered as viable alternative to generative models such as VAEs. More specifically, we have found that the main limitation of BAEs lies in the difficulty of specifying meaningful priors in the context of highly-structured data, which is ubiquitous in modern machine learning applications. Consequently, we have proposed to specify priors over the autoencoder weights by means of a novel optimization of prior hyper-parameters. Inspired by connections with marginal likelihood optimization, we derived a practical and efficient optimization framework, based on the minimization of the distributional sliced-Wasserstein distance between the distribution induced by the BAE and the data generating distribution. The resulting hyper-parameter optimization strategy leads to a novel way to perform model selection for BAEs, and we showed its advantages in an extensive experimental campaign.

**Limitations and ethical concerns.** Even if theoretically justified and empirically verified with extensive experimentation, our proposal for model selection still remains a proxy to the true marginal likelihood maximization. The DSWD formulation has nice properties of asymptotic convergence and computational tractability, but it may represent only one of the possible solutions. At the same time, we stress that the current literature does not cover this problem of BAEs at all, and we believe our approach is a considerable step towards the development of practical Bayesian methods for representation learning in modern applications characterized by large-scale structured data (including tabular and graph data, which are currently not covered). At the same time, the accessibility to these models to a wider audience and different kind of data might help to widespread harmful applications, which is a concern shared among all generative modeling approaches. An ethical analysis of the consequences of Bayesian priors in unsupervised learning scenarios is also worth an in-depth investigation, which goes beyond the scope of this work.
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A Derivation of Distributional Sliced-Wasserstein Distance

In this section, we review some key results on the Wasserstein distance. Given two probability measures $\pi$, $\rho$, both defined on $\mathbb{R}^D$ for simplicity, the $p$-Wasserstein distance between $\pi$ and $\rho$ is given by

$$W_p^p(\pi, \rho) = \inf_{\gamma \in \Gamma(\pi, \rho)} \int \|x - y\|^p \gamma(x, y) \, dx \, dy,$$

where $\Gamma(\pi, \rho)$ is the set of all possible distributions $\gamma(x, y)$ such that the marginals are $\pi(x)$ and $\rho(y)$ [62]. While usually analytically unavailable, for $D = 1$ the distance has the following closed form solution,

$$W_p^p(\pi, \rho) = \int_0^1 |F^{-1}_\pi(z) - F^{-1}_\rho(z)|^p \, dz,$$

where $F_\pi$ and $F_\rho$ are the cumulative density functions (CDFs) of $\pi$ and $\rho$, respectively.

A.1 (Distributional) Sliced-Wasserstein Distance

The main idea underlying the DSWD is to project the challenging estimation of distances for high-dimensional distributions into simpler estimation of multiple distances in one dimension, which all have closed-form solution (Eq. 13). The projection is done using the Radon transform $\mathcal{R}$, an operator that maps a density function $\varphi$ defined in $\mathbb{R}^D$ to the set of its integrals over hyperplanes in $\mathbb{R}^D$,

$$\mathcal{R}\varphi(t, \theta) := \int \varphi(z) \delta(t - z^\top \theta) \, dz, \quad \forall t \in \mathbb{R}, \quad \forall \theta \in S^{D-1},$$

where $S^{D-1}$ is the unit sphere in $\mathbb{R}^D$ and $\delta(\cdot)$ is the Dirac delta [24]. Using the Radon transform, for a given $\theta$ we can project the two densities $\pi$ and $\rho$ into one dimension,

$$W_p^p(\pi, \rho) = \int_{S^{D-1}} W_p^p(\mathcal{R}\pi(t, \theta), \mathcal{R}\rho(t, \theta)) \, d\theta \approx \frac{1}{K} \sum_{i=1}^K W_p^p(\mathcal{R}\pi(t, \theta_i), \mathcal{R}\rho(t, \theta_i)),$$

where the approximation comes from using Monte-Carlo integration by sampling $\theta_i$ uniformly in $S^{D-1}$ [9]. While having significant computational advantages, this approach might require to draw many unimportant projections that are computationally exhausting and that provide a minimal improvement on the overall distance approximation.

The distributional sliced-Wasserstein distance (DSW) [50] solves this issue by finding the optimal probability measure of slices $\sigma(\theta)$ on the unit sphere $S^{D-1}$ and it’s defined as follows,

$$DSW_p^p(\pi, \rho; C) := \sup_{\sigma \in M_C} \left( E_{\sigma(\theta)} W_p^p(\mathcal{R}\pi(t, \theta), \mathcal{R}\rho(t, \theta)) \right)^{1/p},$$

where, for $C > 0$, $M_C$ is the set of probability measures $\sigma$ such that $E_{\theta, \theta' \sim \sigma} \left[ \theta^\top \theta' \right] \leq C$ (a constraint that aims to avoid directions to lie in only one small area). Critically, the definition of DSWD in Eq. 16 does not suffer from the curse of dimensionality, indeed [50] showed that the statistical error of this estimation scales down with $C_D \cdot n^{-\frac{1}{2D}}$, where $C_D$ is a constant depending on dimension $D$. Furthermore, while generally we have that $DSW_p^p(\pi, \rho) \leq W_p^p(\pi, \rho)$, it can be proved that under mild assumptions on $C$, the two distances are topological equivalent, i.e. converging in distribution on $DSW_p^p$ implies the convergence on $W_p^p$ [see Theorem 2 in 50].

The direct computation of $DSW_p^p$ in Eq. 16 is still challenging but it admits an equivalent dual form,

$$\sup_{h \in \mathcal{H}} \left\{ \left( E_{\bar{\sigma}(\theta)} \left[ W_p^p(\mathcal{R}\pi(t, h(\theta)), \mathcal{R}\rho(t, h(\theta))) \right] \right)^{1/p} - \lambda_C E_{\theta, \theta' \sim \bar{\sigma}} \left[ |h(\theta)^\top h(\theta')| \right] \right\} + \lambda_C C,$$

where $\bar{\sigma}$ is a uniform distribution in $S^{D-1}$, $\mathcal{H}$ is a class of all Borel measurable functions $S^{D-1} \rightarrow S^{D-1}$ and $\lambda_C$ is a regularization hyper-parameter. The formulation in Eq. 17 is obtained by employing the Lagrangian duality theorem and by reparameterizing $\sigma(\theta)$ as push-forward transformation of
a uniform measure in \( S^{D-1} \). Now, by parameterizing \( h \) using a deep neural network\(^1\) with parameters \( \phi \), defined as \( h_{\phi} \), Eq. 17 becomes an optimization problem with respect to the network parameters. The final step is to approximate the analytically intractable expectations with Monte Carlo integration,

\[
D_{SW_{p}}(\pi, \rho) \approx \max_{\phi} \left\{ \left[ \frac{1}{K} \sum_{i=1}^{K} W_{p}^{p} \left( R_{\pi}(t, h_{\phi}(\theta_{i})), R_{\rho}(t, h_{\phi}(\theta_{i})) \right) \right]^{1/p} - \frac{\lambda_{C}}{K} \sum_{i,j=1}^{K} |h_{\phi}(\theta_{i}) \cdot h_{\phi}(\theta_{j})| + \lambda_{C} C \right\},
\]

(18)

where \( \theta_{i} \) are uniform samples from the unit sphere \( S^{D-1} \) and \( \forall t \in \mathbb{R} \). Finally, we can use stochastic gradient methods to update \( \phi \) and then use the resulting optima for the estimation of the original distance.

**B Numerical Implementation of Sliced-Wasserstein Distance**

**B.1 Wasserstein distance between two empirical 1D distributions**

The Wasserstein distance between two one-dimensional distributions \( \pi \) and \( \rho \) is defined as in Eq. 13. The integral in this equation can be numerically estimated by using the midpoint Riemann sum:

\[
\int_{0}^{1} |F_{\pi}^{-1}(z) - F_{\rho}^{-1}(z)|^p dz \approx \frac{1}{M} \sum_{m=1}^{M} |F_{\pi}^{-1}(z_m) - F_{\rho}^{-1}(z_m)|^p,
\]

(19)

where \( z_m = \frac{2m-1}{M} \), \( M \) is the number of points used to approximate the integral. If we only have samples from the distributions, \( x_m \sim \pi \) and \( y_m \sim \rho \), we can obtain the empirical densities as follows

\[
\pi(x) \approx \pi_M(x) = \frac{1}{M} \sum_{m=1}^{M} \delta(x - x_m),
\]

(20)

\[
\rho(y) \approx \rho_M(y) = \frac{1}{M} \sum_{m=1}^{M} \delta(y - y_m),
\]

(21)

where \( \delta \) is the Dirac delta function. The corresponding empirical cumulative density functions are

\[
F_{\pi}(z) \approx F_{\pi,M}(z) = \frac{1}{M} \sum_{m=1}^{M} u(z - x_m),
\]

(22)

\[
F_{\rho}(z) \approx F_{\rho,M}(z) = \frac{1}{M} \sum_{m=1}^{M} u(z - y_m),
\]

(23)

where \( M \) is the number of samples, \( u(\cdot) \) is the step function.

Calculating the Wasserstein distance with the empirical distribution function is computationally attractive. To do that, we first sort \( x_m s \) in an ascending order, such that \( x_{i[m]} \leq x_{i[m+1]} \), where \( i[m] \) is the index of the sorted \( x_m s \). It is straightforward to show that \( F_{\pi,M}^{-1}(z_m) = x_{i[m]} \). Thus, the Wasserstein distance can be approximated as follows

\[
W_{p}^{p}(\pi, \rho) \approx \frac{1}{M} \sum_{m=1}^{M} |x_{i[m]} - y_{j[m]}|^p.
\]

(24)

**B.2 Slicing empirical distribution**

According to the equation Eq. 14, the marginal densities (i.e. slices) of the distribution \( \pi \) can be obtained as follows

\[
R_{\pi}(t, \theta) = \int \pi(x) \delta(t - x^{\top} \theta) dx, \quad \forall t \in \mathbb{R}.
\]

(25)

\(^1\)We use a single multi layer perceptron (MLP) layer with normalized output as the \( h \) function.
Because, in practice, only samples from the distributions are available we aim to calculate a Radon slice of the empirical distribution of $M$ samples $\pi_M = \frac{1}{M} \sum_{m=1}^{M} \delta(x - x_m)$:

$$
\mathcal{R} \pi(t, \theta) \approx \frac{1}{M} \sum_{m=1}^{M} \int \delta(x - x_m) \delta(t - x_\top \theta) dx
$$

By using the approximation in Eq. 27 and the empirical implementation of 1D Wasserstein distance (Eq. 24), we are able to compute a proxy to the original distance in Eq. 16.

C Pseudocode of Prior Optimization Procedure
Algorithm 1 describes the procedure of prior optimization for BAES.

Algorithm 1: Prior Optimization

Input: Empirical distribution $\tilde{\pi}(x)$; prior over parameters $p_\psi(w)$; number of prior samples $N_S$; mini-batch size $N_B$; number of random projections $K$; regularization coefficient $\lambda_C$.

Output: The optimized prior’s parameters $\psi$

while $\psi$ has not converged do

Sample $x = \{x_i\}_{i=1}^{N_M}$ from $\tilde{\pi}(x)$ // Sample input data
Sample $W = \{w_i\}_{i=1}^{N_S}$ from $p_\psi(w)$ // Sample parameters from the prior

foreach $w_i \in W$ do

Following steps are performed in a batch manner */

Sample $\tilde{x}_i = f_{\text{dec}}(f_{\text{enc}}(x))$ // Compute the functional outputs from Autoencoder
Sample $\tilde{x}_i$ from $p(x | x_i)$ // Sample from the likelihood
Gather samples $\tilde{x} = \cup \{\tilde{x}_i\}_{i=1}^{N_S}$
$L = DSW_2(\tilde{x}, \tilde{x}; K, \lambda_C)$ // Compute the $DSW_2$ distance using Eq. 18
$\psi \leftarrow \text{Optimizer}(\psi, \nabla_\psi L)$ // Update prior’s parameters

Return: $\psi$

D Details on Stochastic gradient Hamiltonian Monte Carlo

Hamiltonian Monte Carlo (HMC) [49] is a highly-efficient Markov Chain Monte Carlo (MCMC) method used to generate samples from the posterior $w \sim p(w | x)$. HMC considers the joint log-likelihood as a potential energy function $U(w) = -\log p(x | w) - \log p(w)$, and introduces a set of auxiliary momentum variable $r$. Samples are generated from the joint distribution $p(w, r)$ based on the Hamiltonian dynamics:

$$
\begin{align*}
\{dw\} &= M^{-1} r dt, \\
\{dr\} &= -\nabla U(w) dt,
\end{align*}
$$

where, $M$ is an arbitrary mass matrix that plays the role of a preconditioner. In practice, this continuous system is approximated by means of $\varepsilon$-discretized numerical integration, and followed by Metropolis steps to accommodate numerical errors stemming from the integration.

However, HMC is not practical for large datasets due to the cost of computing the gradient $\nabla U(w) = \nabla \log p(x | w)$ on the entire dataset. To mitigate this issue, [11] proposed SGHMC, which uses a noisy, unbiased estimate of the gradient $\nabla U(w)$ which is computed from a mini-batch of the data. The discretized Hamiltonian dynamics are then updated as follows

$$
\begin{align*}
\Delta w &= \varepsilon M^{-1} r, \\
\Delta r &= -\varepsilon \nabla U(w) - \varepsilon C M^{-1} r + N(0, 2\varepsilon (C - \hat{B})),
\end{align*}
$$

where $\varepsilon$ is an step size, $C$ is an user-defined friction matrix, $\hat{B}$ is the estimate for the noise of the gradient evaluation. To choose these hyper-parameters, we use a scale-adapted version of SGHMC [56], where the hyper-parameters are adjusted automatically during a burn-in phase. After this period, all hyperparameters stay fixed.
**Estimating M.** We set the mass matrix $M^{-1} = \text{diag} \left( \hat{V}_w^{-1/2} \right)$, where $\hat{V}_w^{-1/2}$ is an estimate of the uncentered variance of the gradient, $\hat{V}_w^{-1/2} \approx \mathbb{E}[\nabla \hat{U}(w)^2]$, which can be estimated by using exponential moving average as follows

$$\Delta \hat{V}_w = -\tau^{-1} \hat{V}_w + \tau^{-1} \nabla (\hat{U}(w))^2,$$

where $\tau$ is a parameter vector that specifies the moving average windows. This parameter can be automatically chosen by using an adaptive estimate [56] as follows

$$\Delta \tau = -g_w^2 \hat{V}_w^{-1} \tau + 1, \quad \text{and} \quad \Delta g_w = -\tau^{-1} g_w + \tau^{-1} \nabla \hat{U}(w),$$

where $g_w$ is a smoothed estimate of the gradient $\nabla \hat{U}(w)$.

**Estimating $\hat{B}$:** The estimate for the noise of the gradient evaluation, $\hat{B}$ should be ideally the estimate of empirical Fisher information matrix of $U(w)$, which is prohibitively expensive to compute. Therefore, we use a diagonal approximation, $\hat{B} = \frac{1}{2} \epsilon \hat{V}_w$, which is already available from the step of estimating $M$.

**Choosing C.** In practice, one can simply set the friction matrix as $C = CI$, i.e. the same independent noise for each elements of $w$.

**The discretized Hamiltonian dynamics.** By substituting $v := \epsilon \hat{V}_w^{-1/2} r$, the dynamics Eq. 29 become

$$\begin{align*}
\Delta w &= v, \\
\Delta v &= -\epsilon^2 \hat{V}_w^{-1/2} \nabla \hat{U}(w) - \epsilon C \hat{V}_w^{-1/2} v + \mathcal{N}(0, 2\epsilon^3 C \hat{V}_w^{-1} - \epsilon^4 I). 
\end{align*}$$

Following [56], we choose $C$ such that $\epsilon C \hat{V}_w^{-1/2} = \alpha I$. This is equivalent to using a constant momentum coefficient of $\alpha$. The final discretized dynamics are then

$$\begin{align*}
\Delta w &= v, \\
\Delta v &= -\epsilon^2 \hat{V}_w^{-1/2} \nabla \hat{U}(w) - \alpha v + \mathcal{N}(0, 2\epsilon^2 \alpha \hat{V}_w^{-1/2} - \epsilon^4 I). 
\end{align*}$$

**E PCA of the SGD Trajectory**

Inspired by [28], we use the subspace spanned by the SGD trajectory to visualize neural network’s parameters in a low-dimensional space. This subspace is cheap to construct and can capture many of the sharp directions of the loss surface [28, 37, 44]. More specifically, we perform SGD starting from a MAP solution with a constant learning rate. Here, the loss function is the negative log joint likelihood of the BAE:

$$\mathcal{L}(w) = -\frac{N}{M} \sum_{i=1}^{M} \log p(x_i \mid w) - \log p(w),$$

where $M$ is the mini-batch size and $N$ is the size of training data. We store the deviations $\alpha_i = w - w_i$ for the last $M$ epochs, where $w$ is the running average of the first moment. $M$ is determined by the amount of memory we can use. Then we perform PCA based on randomized SVD [23] on the matrix $A$ comprised of vectors $\alpha_1, ..., \alpha_M$ to construct the subspace. The procedure is summarized in Algorithm 2.
Algorithm 2: Subspace construction with PCA

Input: Pretrained paremeters \( w_{\text{MAP}} \); learning rate \( \eta \); number of steps \( T \); momentum update frequency \( c \); maximum number of columns \( M \) in deviation matrix \( A \).

Output: Shift vector \( \overline{w} \); projection matrix \( P \) for subspace.

\[
\begin{align*}
1. & \quad \overline{w} \leftarrow w_{\text{MAP}} \quad // \text{Initialize mean} \\
2. & \quad \text{for } i \leftarrow 1, 2, ..., T \text{ do} \\
3. & \quad \quad w_i \leftarrow w_{i-1} - \eta \nabla_w \mathcal{L}(w_{i-1}) \quad // \text{Perform SGD update} \\
4. & \quad \quad \text{if } \text{MOD}(i, c) = 0 \text{ then} \\
5. & \quad \quad \quad n \leftarrow i/c \quad // \text{Number of models} \\
6. & \quad \quad \quad \overline{w} \leftarrow \frac{n}{n+1} \overline{w} + w_{i+1} \quad // \text{Update mean} \\
7. & \quad \quad \text{if } \text{NUM}_\text{COLS}(A) = M \text{ then} \\
8. & \quad \quad \quad \text{REMOVE}_\text{COL}(A[:,1]) \\
9. & \quad \quad \quad \text{APPEND}_\text{COL}(A, w_i - \overline{w}) \quad // \text{Store deviation} \\
10. & \quad U, S, V^T \leftarrow \text{SVD}(A) \quad // \text{Perform truncated SVD} \\
11. & \quad \text{Return: } \overline{w}, P = SV^T
\end{align*}
\]

F Additional Details on Experimental Settings

F.1 Experimental environment

In our experiments, we use 4 workstations, which have the following specifications:

- **GPU**: NVIDIA Tesla P100 PCIe 16 GB.
- **CPU**: Intel(R) Xeon(R) (4 cores) @ 2.30GHz.
- **Memory**: 25.5 GiB (DDR3).

F.2 Preprocessing data

- **MNIST [36]**: The dataset is publicly available at [http://yann.lecun.com/exdb/mnist](http://yann.lecun.com/exdb/mnist). We keep the original resolution of 1 × 28 × 28 of the MNIST dataset.

- **FREY-YALE [15]**: The FREY and YALE datasets are publicly available at [http://cs.nyu.edu/~roweis/data.html](http://cs.nyu.edu/~roweis/data.html) and [http://vision.ucsd.edu/extyaleb/CroppedYaleBZip](http://vision.ucsd.edu/extyaleb/CroppedYaleBZip), respectively. All the images of FREY and YALE datasets are resized to the 1 × 28 × 28 resolution.

- **CELEBA [38]**: The dataset is publicly available at [http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html](http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html). According to [17], we pre-process CELEBA images by first taking a 148 × 148 center crop and then resizing to the 3 × 64 × 64 resolution.

F.3 Network architectures

In our experiments, we use convolutional networks for modeling both encoders and decoders. For a fair comparison, we employ the same network architecture for all models. The network’s parameters are initialized by using the default scheme in PyTorch [53].

Table 1 shows details on the network architectures used in our experimental campaign.
whereas

| Table 1: Convolutional Encoder-Decoder architectures. | Convolutional Encoder-Decoder architectures. |
|---------------------------------|---------------------------------|
| **MNIST** | **FREY-YALE** | **CELEBA** |
| Encoder: | Encoder: | Encoder: |
| $x \in \mathbb{R}^{1 \times 28 \times 28}$ | $x \in \mathbb{R}^{1 \times 28 \times 28}$ | $x \in \mathbb{R}^{3 \times 64 \times 64}$ |
| $\rightarrow \text{Conv}_{32} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{256} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{256} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{512} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{512} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{FLATTEN} \rightarrow \text{FC}_{50 \times M}$ | $\rightarrow \text{FLATTEN} \rightarrow \text{FC}_{50 \times M}$ | $\rightarrow \text{FLATTEN} \rightarrow \text{FC}_{50 \times M}$ |

| Decoder: | Decoder: | Decoder: |
|---------------------------------|---------------------------------|
| $z \in \mathbb{R}^{50} \rightarrow \text{FC}_{7 \times 7 \times 128}$ | $z \in \mathbb{R}^{50} \rightarrow \text{FC}_{7 \times 7 \times 256}$ | $z \in \mathbb{R}^{50} \rightarrow \text{FC}_{8 \times 8 \times 512}$ |
| $\rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{256} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{256} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{64} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{512} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{512} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ | $\rightarrow \text{Conv}_{128} \rightarrow \text{LEAKY RELU}$ |
| $\rightarrow \text{CONV}_{T_{1}} \rightarrow \text{SIGMOID}$ | $\rightarrow \text{CONV}_{T_{1}} \rightarrow \text{SIGMOID}$ | $\rightarrow \text{CONV}_{T_{1}} \rightarrow \text{SIGMOID}$ |

Table 1: Convolutional Encoder-Decoder architectures. Conv. denotes a convolutional layer with n filters, whereas Conv. represents a fully-connected layer with n units. All convolutions and transposed convolutions have a filter size of 4x4 for MNIST and FREY-YALE and 5x5 for CELEBA. M = 1 for all models except for the VAEs which have M = 2 as the encoder has to yield both mean and variance for each input.

F.4 Prior optimization

As done in [50], we use a single-layer multilayer perceptron (MLP), $h_\phi$, to represent the Borel measurable function in the dual form of DSWD (Eq. 18). At each iteration of Algorithm 1, to find a local maxima, we optimize $h_\phi$ for 30 epochs by using an Adam optimizer [31] with a learning rate of 0.0005. We use another Adam optimizer with a learning rate of 0.001 to update the prior’s parameters. We use a mini-batch size of $N_B = 64$ and then generate $N_s = 32$ prior samples given each data point. By default, we use $K = 1000$ random projections with a regularization coefficient $\lambda_C = 100$ to estimate the 2-Wasserstein distance. The convergences of prior optimization on MNIST, FREY and CELEBA datasets are illustrated in Fig. 16.

F.5 SGHMC hyper-parameters

In Table 2 we report the hyper-parameters used in the experiments on MNIST, YALE and CELEBA datasets. As seen, we always use a fixed step size of 0.003, a momentum coefficient of 0.05, and a mini-batch size of 64. The number of collected samples after thinning is 32. The number of burn-in iterations and the thinning interval are increased according to the size of the training set.

| Training Size | MNIST | YALE | CELEBA |
|---------------|-------|------|--------|
| **MINI-BATCH SIZE** | 64 | 64 | 64 |
| **STEP SIZE (10^-3)** | 3 | 3 | 3 |
| **MOMENTUM (10^-2)** | 5 | 5 | 5 |
| **NUM. BURN-IN STEPS (10^3)** | 6 | 6 | 6 |
| **NUM. SAMPLES** | 32 | 32 | 32 |
| **THINNING INTERVAL (10^3)** | 1 | 1 | 1 |

Table 2: SGHMC hyper-parameters used in the experiments on MNIST, YALE and CELEBA datasets.

F.6 Competing approaches

- **VAE [32]**: The vanilla VAE model employed with a Gaussian encoder and a standard Gaussian prior on the latent space.

- **β-VAE [26]**: The KL term in the VAE’s objective is weighted by $\beta = 0.1$ to reduce the effect of the prior. This helps to avoid the over-regularization problem of VAEs and improve reconstruction quality.

- **VAE + Sylvester Flows [61]**: One of the state-of-the-art normalizing flows for the encoder of VAEs, which has richer expressiveness than VAE’s post-Gaussian encoder. As employed in [61], we use Orthogonal Sylvester flows with 4 transformations and 32 orthogonal vectors.
• **VAE + VampPrior** [59]: A flexible prior for VAEs, which is a mixture of variational posteriors conditioned on learnable pseudo-observations. This allows the variational posterior to learn more a potential latent representation. Due to using small training data, we use 100 trainable pseudo-observations in our experiments. We found that increasing more pseudo-observations may hurt the predictive performance because of overfitting.

• **2-Stage VAE** [14]: A simple and practical method to improve the quality of generated images from VAEs by performing a form of ex-post density estimation via a second VAE. As employed in [14], for the second-stage VAE, we use a MLP having three 1024-dimensional hidden layers with ReLU activation function.

• **WAE** [58] Wasserstein Autoencoder: This model is an alternative of VAEs. By reformulating the objective function as an OT problem, WAE regularizes the averaged encoding distribution instead of each data point. This encourages the encoded training distribution to match the prior while still allowing to learn significant information from the data. As suggested in [58], we use WAE-MMD with the inverse multiquadratics kernel and a regularization coefficient $\lambda = 10$ due to its stability compared to WAE-GAN. We impose the standard Gaussian prior on the latent space.

• **NS-GAN** [21]: a standard GAN with the non-saturating loss, which has been shown to be robust to the choice of hyper-parameters on CELEBA [40]. For a fair comparison, we reuse the encoder and decoder architectures for the discriminator and generator, respectively.

• **DiffAugment-GAN** [69]: a more complex architecture [STYLEGAN2, see 30] combined with a powerful differentiable augmentation scheme, specifically developed for low data regimes. We refer to the original work of [69] and the implementation in https://github.com/mit-han-lab/data-efficient-gans for additional details on the network architecture. We use the same latent size of 50, a maximum of 64 feature maps, and all available augmentations (color, cutout and translation). The remaining parameters are left at default value.

All autoencoder models are trained for 200 epochs with an Adam optimizer [31] using the default hyper-parameters in PyTorch, i.e. learning rate $= 0.001$, $\beta_1 = 0.9$, $\beta_2 = 0.999$. The NS-GAN is trained for 200 epochs with a learning rate of 0.0002. The DiffAugment-GAN is trained with learning rate of 0.001 for 1 million steps (expect for the case of 4000 training samples, which was extended for 2 millions steps).

### F.7 Performance evaluation

#### Test log-likelihood.

To evaluate the reconstruction quality, we use the mean predictive log-likelihood evaluated over the test set. This metric tells us how probable it is that the test targets were generated using the test inputs and our model. Notice that for the case of autoencoder models, the test targets are exactly the test inputs. The predictive likelihood is a proper scoring rule [20] that depends on both the accuracy of predictions and their uncertainty.

For BAE, as done in the literature of BNNS [29, 52], we can estimate the predictive likelihood for an unseen datapoint, $x^*$, as follows

$$E_{p(w \mid x)}[p(x^* \mid w)] \approx \frac{1}{M} \sum_{i=1}^{M} p(x^* \mid w_i), \quad w_i \sim p(w \mid x),$$

where $w_i$ is a sample from the posterior $p(w \mid x)$ obtained from the SGHMC sampler.

For VAEs, because the randomness comes from the latent code not the network’s parameters, we can use MC approximation to estimate the predictive likelihood as follows

$$E_{q(z \mid x^*)}[p(x^* \mid z)] \approx \frac{1}{N} \sum_{i=1}^{N} p(x^* \mid z_i), \quad z_i \sim q(z \mid x^*),$$

where $q(z \mid x^*)$ is the amortized approximate posterior. In our experiments, we use $N = 200$. 

20
For completeness, we also report the test marginal log-likelihood $p(x)$ of VAEs, which is estimated by the importance weighted sampling (IWAE) method [10]. More specifically,

$$
\text{IWAE} = \log \left( \frac{1}{K} \sum_{i=1}^{K} p(x^*, z_i) \right), \quad z_i \sim q(z | x^*).
$$

It can be shown that IWAE lower bounds $\log p(x^*)$ and can be arbitrarily close to the target as the number of samples $K$ grows. We use $K = 1000$ in the experiments. The full results of test marginal log-likelihood are reported in Tables 7, 8 and 9.

**FID score.** To assess the quality of the generated images, we employed the widely used Fréchet Inception Distance [25]. This metric is the Fréchet distance between two multivariate Gaussians, the generated samples and real data samples are compared through their distribution statistics:

$$
\text{FID} = \|\mu_{\text{real}} - \mu_{\text{gen}}\|^2 + \text{Tr}(\Sigma_{\text{real}} + \Sigma_{\text{gen}} - 2\sqrt{\Sigma_{\text{real}}\Sigma_{\text{gen}}}).
$$

Two distribution samples are calculated from the 2048-dimensional activations of pool3 layer of Inception-v3 network \(^2\). In our experiments, the statistics of generated and real data are computed over 10000 generated images and test data, respectively.

\(^2\)We use the original TensorFlow implementation of FID score which is available at https://github.com/bioinf-jku/TTUR.


G Additional Results of Comparison with Temperature Scaling

In Bayesian deep learning, temperature scaling is a practical technique to improve predictive performance [28, 63, 67]. There are two main approaches to tempering the posterior, namely (1) partial tempering and (2) full tempering [1, 66]. In this section, we investigate rigorously the posteriors induced by the \( \mathcal{N}(0, 1) \) prior and optimized prior under different tempering settings. We use the same setup of MNIST as in the main paper, with 200 examples for inference. For the optimized prior, we use 100 training samples for learning prior. For the \( \mathcal{N}(0, 1) \) prior, we use the union of 200 training samples and the data used to optimized prior for training.

G.1 Partial Tempering

The partially tempered posterior is defined as follows [28, 64]

\[
\hat{p}_{\text{tempered}}(\mathbf{w} | \mathbf{x}) \propto \frac{p(\mathbf{x} | \mathbf{w})^{1/\tau}}{p(\mathbf{w})},
\]

where \( \tau > 0 \) is a temperature value. This parameter controls how the prior and likelihood interact in the posterior. When \( \tau = 1 \) the true posterior is recovered, and as \( \tau \) becomes large, the tempered posterior approaches the prior. In the case of small training data and using a misspecified prior such as \( \mathcal{N}(0, 1) \), we would use a small temperature value (e.g. \( \tau < 1 \)) to reduce the effect of the prior. This corresponds to artificially sharpening the posterior by overcounting the data by a factor of \( \tau \).

Fig. 9 shows the test LL on MNIST for BAE with \( \mathcal{N}(0, 1) \) prior and different temperature values. As expected, the predictive performance of the posterior obtained via low temperatures \( \tau < 1 \) is much better than those at high temperatures \( \tau > 1 \). However, cooling the posterior only shows slight improvement compared to the true posterior induced from the optimized prior. In addition, in case \( \tau > 1 \), where the influence of the posterior becomes stronger, the tempered posterior w.r.t. the optimized prior is significantly better than using the \( \mathcal{N}(0, 1) \) prior. This again shows clearly that \( \mathcal{N}(0, 1) \) is a poor prior for a deep BAE.

Fig. 10a illustrates samples from priors and posteriors in a low-dimensional space. We also consider the posterior obtained from the entire training data and the \( \mathcal{N}(0, 1) \) prior as “oracle” posterior. In this case, the choice of the prior does not strongly affect the posterior as this is dominated by the likelihood. It can be seen that, for high-temperature values \( \tau > 1 \), the warm posteriors w.r.t. \( \mathcal{N}(0, 1) \) prior are stretched out as the prior effect is too strong. These posteriors are mismatched with the “oracle” posterior as further confirmed by very low test log-likelihood. Meanwhile, due to the good inductive bias from the optimized prior, the corresponding tempered posterior is still located in regions nearby the “oracle” posterior. For low temperature values \( \tau < 1 \), the cold posteriors are more concentrated by overcounting evidence. However, if we use a very small temperature (e.g. \( \tau = 10^{-4} \)), the resulting posterior overly concentrates around the MLE, becoming too constrained by the training data.

![Figure 9](image-url)  
**Figure 9:** Test LL as a function of temperature on MNIST using BAE with \( \mathcal{N}(0, 1) \) prior. The dotted lines indicate the best performance of LL.

\[\tau \leq 1\]

\[\tau > 1\]
G.2  Full Tempering

For the fully tempered posterior, instead of scaling the likelihood term only, we scale the whole posterior as follows

\[ p_{\tau_{\text{full}}} (w \mid x) \propto \left( \frac{p(x \mid w) \cdot p(w)}{\text{likelihood \ prior}} \right)^{1/\tau}. \]

The only difference between partial and full tempering is whether we scale the prior. If we place Gaussian priors on the parameters, this scaling can be absorbed into the prior variance, \( \sigma^2_{\text{full}} = \sigma^2_{\text{partial}} / \tau \).

Recently, [63] argues that BNNs require a cold posterior, where \( \tau < 1 \) is employed, to obtain a good performance. However, we hypothesize that the cold posterior effect may originate from using a poor prior. In this case, as shown in Fig. 9b, the results of full tempering are similar to those of partial tempering. Cooling the posterior only helps to increase slightly predictive performance for \( \mathcal{N}(0, 1) \) prior. We also observe that the MCMC sampling is not converged if a very large \( \tau \) is employed, thus we only consider small values of \( \tau \) (e.g. \( \tau \in \{5, 10\} \)). In these cases, as depicted in Fig. 10b, the samples from the posterior may be outside of the hypothesis space of the optimized prior.

In sum, the true posterior induced from our optimized prior is remarkably better than any types of tempered posteriors. These results suggest that, in the small-data regime, we should choose carefully a more sensible prior rather than simply using a vague prior and overcounting the data.
Figure 10: Visualization of samples from priors and posteriors of BAE’s parameters in the plane spanned by eigenvectors of the SGD trajectory. ♦ indicates using 200 samples for training; ⋆ indicates using the union of these samples and 100 samples used for learning the prior; ■ denotes using all 60000 training samples. Here, τ is the temperature value used for the ♦ and ⋆ cases. All plots are produced using convolutional BAE on MNIST.
H Ablation Studies

H.1 Additional results of ablation study on the size of the dataset to optimize priors

In this experiment, we demonstrate that we can obtain a sensible result by using a small number of training instances to optimize the prior. Here, we use a set of 200 samples of 0-9 digits for inference, and another dataset also consisting of 0-9 digits for optimizing the prior. Fig. 13 shows the predictive performance and samples from the posterior. We observe that the performance gain by using more data is not significant. We can achieve sensible results by using only about 10-50 samples for each class. In addition, as illustrated in the low-dimensional space (Fig. 13), the hypothesis space of the prior is not collapsed as we increase the size of the dataset used to optimize the prior. As a result, the predictive posterior is also not concentrated to the MLE solutions as further demonstrated in Fig. 12. This behavior is very different from overcounting the data by using temperature scaling, where the posterior becomes more concentrated as the temperature is decreased. This again demonstrates the practicality of our proposed method in the small-data regime.

H.2 Effect of the dimensionality of latent space

Fig. 11 illustrates the predictive performance of VAEs and BAES in terms test LL on MNIST for different size of the latent space and training size. It is clear that BAES with optimized prior consistently outperforms other competitors across all dimensionalities of the latent space and training sizes.

![Figure 11: Ablation study on the test LL on MNIST dataset for different sizes of the latent space and training sizes.](image)

H.3 Visualizing 2-dimensional latent space

We run several experiments with a low latent space ($K = 2$) to test the efficacy of VAEs and BAES as dimensionality reduction techniques. Fig. 14 shows the results, where each color represents an MNIST digit. As seen, BAES with optimized prior produces a more well-defined class structure in comparison with other methods.

We also consider the 2D latent space to visualize that ex-post density estimation with DPMM helps to reduce the mismatch between the aggregated posterior and the prior. As can be seen from Fig. 15, there are large mismatches between aggregated posterior of VAEs and the $N(0, 1)$ prior. We can reduce this problem by using a more expressive prior like VampPrior, or performing ex-post density estimation with a second VAE. For BAES, it is clear that the flexible DPMM estimator effectively fixes the mismatch and this results in better sample quality as reported in the main paper.
Figure 12: The average predictive variance computed over test datapoints as a function of (a) the number of data points used to optimize prior, and (b) the temperature used for cooling the posterior. Here, we use 200 datapoints from MNIST dataset for inference. In figure (a), we use the optimized prior and consider the true posterior without any tempering. In figure (b), we use the standard Gaussian prior and employ partial tempering for the posterior.

Figure 13: Visualization of convergence Wasserstein optimization, and samples from priors and posteriors of BAE’s parameters in the plane spanned by eigenvectors of the SGD trajectory corresponding to the first and second largest eigenvalues. Here, $|\mathcal{M}|$ is the size of dataset used for optimizing the prior; ♦ indicates using 200 training samples for inference; ■ denotes using all 60000 training samples for inference; LL denotes the test log-likelihood performance of the posterior w.r.t. the optimized prior. All plots are produced using convolutional BAE on MNIST.
Figure 14: Visualization of 2D latent spaces of variants of autoencoders on MNIST test set where each color represents a digit class. We consider only 5 classes for easier visualization and comparison. All models are trained on 1000 training samples from MNIST dataset.

Figure 15: Different priors and density estimations on the 2-dimensional latent space of VAEs and BAEs. All models are trained on 1000 training samples from MNIST dataset. The gray points are test set samples while the red ones are samples from priors / density estimators. Here, we employ the isotropic Gaussian prior on the latent space of WAE, VAE, β-VAE and VAE with Sylvester Flows. The VampPrior is learned to explicitly model the aggregated posterior while 2-Stage VAE uses another VAE to estimate the density of the learned latent space. Meanwhile, for BAEs, we use DPPMMs for ex-post density estimation.
I Additional Results

I.1 Convergence of Wasserstein optimization

Fig. 16 depicts the progressions of Wasserstein optimization in the MNIST, FREY-YALE and CELEBA experiments.

Figure 16: Convergence of Wasserstein optimization. The shaded areas represent the standard deviation computed over 4 random data splits.
1.2 Tabulated results

Detailed results on MNIST, YALE and CELEBA datasets are reported from Table 3 to Table 9.

### Table 3: Evaluation of all methods in terms of test log-likelihood (the higher, the better) on MNIST. The parentheses are the standard deviations. ★ indicates that we use the union of the training data and the data used to optimize prior to train the model.

| Training Size | 200   | 500   | 1000  | 2000  |
|---------------|-------|-------|-------|-------|
| WAE           | 1590.0 (11.0) | 1732.7 (19.2) | 1809.5 (11.1) | 1857.4 (4.8) |
| ★ WAE         | 1675.2 (10.6) | 1779.6 (10.2) | 1839.3 (6.1)  | 1871.1 (3.1)  |
| VAE           | 1635.1 (8.0)  | 1744.6 (4.5)  | 1805.5 (4.8)  | 1847.1 (3.7)  |
| ★ VAE         | 1697.0 (9.9)  | 1776.2 (6.8)  | 1829.5 (2.8)  | 1849.9 (4.4)  |
| β-VAE         | 1626.2 (10.3) | 1749.7 (9.2)  | 1812.8 (3.8)  | 1862.3 (4.9)  |
| ★ β-VAE       | 1698.2 (8.0)  | 1780.2 (9.3)  | 1841.2 (3.4)  | 1871.9 (4.4)  |
| VAE + SYLVESER | 1635.4 (6.1)  | 1743.5 (1.5)  | 1799.1 (5.5)  | 1836.3 (7.2)  |
| ★ VAE + SYLVESER | 1711.4 (3.0)  | 1781.0 (2.9)  | 1816.7 (6.2)  | 1848.1 (6.5)  |
| VAE + SLYVESER FLOWS | 1699.9 (22.0) | 1742.6 (18.4) | 1799.1 (5.5)  | 1836.3 (7.2)  |
| ★ VAE + SLYVESER FLOWS | 1708.8 (21.2) | 1754.3 (15.8) | 1801.0 (4.3)  | 1838.2 (6.5)  |
| BAE + N(0, 1) PRIOR | 1609.6 (14.4) | 1732.1 (14.2) | 1798.1 (5.4)  | 1839.3 (4.0)  |
| ★ BAE + N(0, 1) PRIOR | 1681.2 (24.5) | 1798.6 (22.8) | 1827.0 (35.9) | 1842.2 (37.4) |
| BAE + OPT. PRIOR (Ours) | 1743.5 (12.0) | 1845.1 (1.2)  | 1879.1 (6.3)  | 1906.8 (1.1)  |

Table 4: Evaluation of all methods in terms of test log-likelihood (the higher, the better) on YALE. The same interpretation as Table 3.

| Training Size | 50    | 100   | 200   | 500   |
|---------------|-------|-------|-------|-------|
| WAE           | 689.7 (10.4)  | 724.8 (4.4)  | 754.5 (3.9)  | 787.0 (0.7)  |
| ★ WAE         | 718.4 (0.9)   | 740.6 (4.6)  | 765.7 (2.2)  | 794.3 (1.6)  |
| VAE           | 692.3 (8.4)   | 723.5 (2.8)  | 738.4 (3.2)  | 774.1 (1.3)  |
| ★ VAE         | 701.2 (5.9)   | 728.2 (3.5)  | 749.4 (2.0)  | 774.8 (2.1)  |
| β-VAE         | 707.1 (5.7)   | 733.8 (8.5)  | 761.1 (3.4)  | 791.8 (0.7)  |
| ★ β-VAE       | 712.1 (7.6)   | 737.8 (4.7)  | 763.4 (1.3)  | 790.8 (1.5)  |
| VAE + SYLVESER | 705.4 (4.8)   | 729.3 (4.4)  | 738.2 (3.2)  | 776.8 (0.9)  |
| ★ VAE + SYLVESER | 682.1 (11.7)  | 716.3 (4.3)  | 739.6 (2.1)  | 765.3 (1.2)  |
| VAE + VAMPRIOR | 690.0 (6.9)   | 722.8 (1.9)  | 740.6 (1.8)  | 766.8 (2.7)  |
| ★ VAE + VAMPRIOR | 691.7 (6.1)   | 716.9 (4.7)  | 737.8 (5.3)  | 764.2 (2.2)  |
| BAE + N(0, 1) PRIOR | 426.1 (27.6)  | 668.8 (12.8) | 724.9 (21.2) | 775.5 (4.6)  |
| ★ BAE + N(0, 1) PRIOR | 388.0 (13.6)  | 570.4 (9.1)  | 688.2 (5.1)  | 752.5 (1.0)  |
| BAE + OPT. PRIOR (Ours) | 730.3 (3.0)   | 754.3 (3.1)  | 771.6 (3.0)  | 793.5 (2.0)  |
| Training Size | Log Likelihood (↑) |
|---------------|--------------------|
| WAE 5732.6 (35.3) | 6266.4 (73.4) | 6703.6 (24.9) | 6928.3 (32.5) |
| ☆ WAE 6509.7 (49.2) | 6659.8 (36.4) | 6864.0 (23.7) | 7021.6 (24.3) |
| VAE 5914.2 (78.3) | 6406.4 (39.6) | 6683.6 (87.5) | 6976.4 (11.9) |
| ☆ VAE 6460.1 (33.7) | 6694.1 (63.1) | 6831.8 (97.2) | 7039.5 (36.5) |
| β-VAE 5710.2 (49.0) | 6192.5 (91.9) | 6406.0 (139.4) | 7000.9 (7.9) |
| ☆ β-VAE 6445.3 (94.0) | 6654.6 (44.5) | 6859.0 (39.8) | 7007.7 (86.3) |
| VAE + SYLVESTER FLOWS 5481.6 (108.4) | 5984.2 (37.4) | 6415.5 (33.5) | 6699.9 (46.9) |
| ☆ VAE + SYLVESTER FLOWS 6241.3 (149.2) | 6437.2 (58.2) | 6519.9 (88.5) | 6831.5 (121.2) |
| VAE + VAMPPRIOR 5776.6 (95.9) | 6242.2 (92.2) | 6691.5 (24.4) | 6999.7 (15.9) |
| ☆ VAE + VAMPPRIOR 6531.7 (61.5) | 6591.6 (97.4) | 6868.3 (27.8) | 6990.7 (37.3) |
| 2-STAGE VAE 5914.2 (78.3) | 6406.4 (39.6) | 6683.6 (87.5) | 6976.4 (11.9) |
| ☆ 2-STAGE VAE 6460.1 (33.7) | 6694.1 (63.1) | 6831.8 (97.2) | 7039.5 (36.5) |
| BAE + N(0, 1) PRIOR 5581.9 (70.8) | 6273.3 (54.2) | 6848.3 (15.1) | 7154.5 (15.6) |
| ☆ BAE + N(0, 1) PRIOR 6531.7 (61.5) | 6591.6 (97.4) | 6868.3 (27.8) | 6990.7 (37.3) |
| BAE + OPTIM. PRIOR (Ours) 6781.3 (32.4) | 7065.8 (15.0) | 7244.7 (8.7) | 7370.0 (13.2) |

Table 5: Evaluation of all methods in terms of test log-likelihood (the higher, the better) on CELEBA. The same interpretation as Table 3.

| Training Size | FID (↓) |
|---------------|---------|
| WAE 342.14 (19.02) | 309.79 (12.58) | 275.10 (8.71) | 253.06 (5.52) |
| ☆ WAE 294.26 (8.41) | 276.24 (10.49) | 261.64 (6.08) | 246.92 (3.28) |
| VAE 271.70 (5.12) | 240.69 (3.44) | 230.61 (7.05) | 209.08 (6.28) |
| ☆ VAE 2460.1 (12.20) | 237.29 (12.48) | 231.50 (14.17) | 206.92 (9.91) |
| β-VAE 323.00 (10.88) | 295.54 (12.45) | 276.71 (15.61) | 260.51 (5.30) |
| ☆ β-VAE 285.81 (5.58) | 277.44 (12.97) | 271.82 (6.69) | 262.72 (17.92) |
| VAE + SYLVESTER FLOWS 221.71 (10.50) | 214.94 (12.01) | 207.86 (9.93) | 198.94 (10.10) |
| ☆ VAE + SYLVESTER FLOWS 210.24 (3.48) | 215.00 (5.79) | 204.42 (11.86) | 179.26 (49.53) |
| VAE + VAMPPRIOR 144.41 (16.61) | 131.02 (2.22) | 112.82 (4.05) | 96.20 (2.79) |
| ☆ VAE + VAMPPRIOR 120.02 (8.62) | 120.23 (7.16) | 102.67 (7.61) | 95.95 (4.86) |
| 2-STAGE VAE 78.23 (2.56) | 69.37 (2.39) | 67.69 (1.55) | 74.47 (4.52) |
| ☆ 2-STAGE VAE 72.21 (3.05) | 69.25 (3.32) | 72.64 (4.62) | 84.95 (3.91) |
| NS-GAN 252.33 (27.03) | 171.18 (15.51) | 205.05 (97.46) | 128.29 (3.81) |
| ☆ NS-GAN 151.28 (2.27) | 150.74 (4.39) | 137.64 (4.14) | 139.43 (8.77) |
| DIFFAUGMENT-GAN 66.09 (0.27) | 58.76 (0.17) | 50.22 (2.62) | 45.14 (0.13) |
| BAE + N(0, 1) PRIOR 89.36 (4.56) | 81.31 (2.50) | 72.50 (1.37) | 71.85 (0.17) |
| ☆ BAE + N(0, 1) PRIOR 86.03 (3.53) | 75.86 (6.45) | 71.21 (1.41) | 70.72 (0.39) |
| BAE + OPTIM. PRIOR (Ours) 68.59 (3.08) | 66.11 (0.96) | 68.34 (0.86) | 67.18 (0.80) |

Table 6: Evaluation of all methods in terms of FID (the lower, the better) on CELEBA. The same interpretation as Table 3.
### Table 7: Evaluation of all methods in terms of test log marginal likelihood of VAE models *(the higher, the better)* on MNIST. The same interpretation as Table 3.

| Training Size | VAE  | β-VAE | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-------|-----------------------|------------------|
| 200           | 1648.2 (10.1) | 1497.1 (12.5) | 1627.0 (6.9) | 1545.6 (10.5) |
| 500           | 1744.0 (5.6)  | 1625.9 (7.7)  | 1709.8 (1.8) | 1681.7 (6.9) |
| 1000          | 1795.1 (2.6)  | 1687.3 (3.8)  | 1741.8 (2.5) | 1737.5 (3.4) |
| 2000          | 1829.7 (2.5)  | 1715.2 (2.9)  | 1771.4 (2.5) | 1795.4 (3.2) |

| Training Size | VAE  | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-----------------------|------------------|
| 50            | 1648.2 (10.1) | 1627.0 (6.9) | 1681.7 (20.2) |
| 100           | 1744.0 (5.6)  | 1709.8 (1.8) | 1741.8 (2.5) |
| 200           | 1795.1 (2.6)  | 1741.8 (2.5) | 1771.4 (2.5) |
| 500           | 1829.7 (2.5)  | 1741.8 (2.5) | 1771.4 (2.5) |

### Table 8: Evaluation of all methods in terms of test log marginal likelihood *(the higher, the better)* of VAE models on YALE. The same interpretation as Table 3.

| Training Size | VAE  | β-VAE | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-------|-----------------------|------------------|
| 50            | 693.8 (7.8)  | 628.1 (2.7)  | 668.6 (5.2)  | 672.7 (7.9) |
| 100           | 720.8 (3.4)  | 655.2 (9.9)  | 686.5 (3.4) | 697.4 (6.8) |
| 200           | 734.5 (2.8)  | 683.0 (3.9)  | 701.2 (2.7) | 721.5 (4.0) |
| 500           | 767.2 (0.6)  | 712.5 (1.6)  | 731.5 (2.3) | 736.8 (4.1) |

| Training Size | VAE  | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-----------------------|------------------|
| 50            | 704.2 (5.6)  | 658.5 (13.4) | 672.7 (7.9) |
| 100           | 723.7 (3.1)  | 683.9 (5.4)  | 697.2 (2.7) | 721.5 (4.0) |
| 200           | 742.4 (1.9)  | 707.2 (2.7)  | 731.5 (2.3) | 736.8 (4.1) |
| 500           | 765.1 (1.2)  | 712.5 (1.6)  | 731.5 (2.3) | 736.8 (4.1) |

### Table 9: Evaluation of all methods in terms of test log marginal likelihood *(the higher, the better)* of VAE models on CELEBA. The same interpretation as Table 3.

| Training Size | VAE  | β-VAE | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-------|-----------------------|------------------|
| 500           | 5973.4 (66.7) | 5496.0 (52.9) | 5545.8 (97.8) | 5842.2 (82.8) |
| 1000          | 6416.6 (36.6) | 6007.8 (89.8) | 5988.2 (40.9) | 6273.8 (86.3) |
| 2000          | 6673.7 (82.6) | 6457.8 (147.2) | 6387.9 (37.8) | 6682.6 (16.8) |
| 4000          | 6943.4 (8.7)  | 6820.1 (7.4)  | 6649.9 (47.1) | 6984.6 (7.4) |

| Training Size | VAE  | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-----------------------|------------------|
| 500           | 6470.0 (30.7) | 6294.4 (98.1) | 6584.3 (98.1) |
| 1000          | 6676.7 (57.4) | 6472.2 (46.1) | 6680.5 (42.8) |
| 2000          | 6807.6 (89.3) | 6648.2 (46.1) | 6680.5 (42.8) |
| 4000          | 7001.2 (37.5) | 6820.1 (7.4)  | 6648.4 (93.9) | 6966.1 (28.0) |

| Training Size | VAE  | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-----------------------|------------------|
| 500           | 5973.4 (66.7) | 5496.0 (52.9) | 5842.2 (82.8) |
| 1000          | 6416.6 (36.6) | 6007.8 (89.8) | 6273.8 (86.3) |
| 2000          | 6673.7 (82.6) | 6457.8 (147.2) | 6682.6 (16.8) |
| 4000          | 6943.4 (8.7)  | 6820.1 (7.4)  | 6984.6 (7.4) |

| Training Size | VAE  | VAE + Sylvestor Flows | VAE + VAMP Prior |
|---------------|------|-----------------------|------------------|
| 500           | 6470.0 (30.7) | 6294.4 (98.1) | 6584.3 (98.1) |
| 1000          | 6676.7 (57.4) | 6472.2 (46.1) | 6680.5 (42.8) |
| 2000          | 6807.6 (89.3) | 6648.2 (46.1) | 6680.5 (42.8) |
| 4000          | 7001.2 (37.5) | 6820.1 (7.4)  | 6648.4 (93.9) | 6966.1 (28.0) |
1.3 More qualitative results

Figure 17: Qualitative evaluation for sample quality for autoencoders and GANs on Celeba. Here, we use 500 samples for training/inference.
Table 10: Qualitative evaluation for reconstructed samples on CELEBA. ⭐ indicates that we use the union of the training data and the data used to optimize prior to train the model. Here, the training size is 1000.

Table 11: Qualitative evaluation for reconstructed samples on MNIST. ⭐ indicates that we use the union of the training data and the data used to optimize prior to train the model. Here, the training size is 200.
Table 12: Qualitative evaluation for generated samples on MNIST. ★ indicates that we use the union of the training data and the data used to optimize prior to train the model. Here, the training size is 200.
Table 13: Qualitative evaluation for reconstructed samples on YALE. ★ indicates that we use the union of the training data and the data used to optimize prior to train the model. Here, the training size is 500.
Table 14: Qualitative evaluation for generated samples on YALE. ★ indicates that we use the union of the training data and the data used to optimize prior to train the model. Here, the training size is 500.