Do Bayesian Variational Autoencoders Know What They Don't Know?

Abstract

The problem of detecting the out-of-distribution (OoD) inputs is of prominent importance for deep neural networks (DNNs). It has been previously shown that even deep generative models (DGMs) that allow estimating the density of the inputs may not be reliable and often tend to make over-confident predictions for OoDs, assigning to them a higher density than to the in-distribution data. This over-confidence of a single model can be potentially mitigated with Bayesian inference over the model parameters that take into account epistemic uncertainty. In this paper, we investigate three different approaches to Bayesian inference: stochastic gradient Markov chain Monte Carlo, Bayes by backprop, and Stochastic Weight Averaging-Gaussian. The inference is implemented over the weights of the deep neural networks that parameterize the likelihood of the variational autoencoder (VAE). We empirically evaluate the approaches against several benchmarks that are often used for OoD detection: estimation of the marginal likelihood utilizing sampled model ensemble, typicality test, disagreement score, and Watanabe-Akaike Information Criterion. Finally, we introduce a simple test based on the idea of the information entropy that demonstrates the state-of-the-art performance.

1 INTRODUCTION

Deep neural networks (DNNs) are trained by maximizing the likelihood estimate (MLE) over parameters $\boldsymbol{\theta}$ given the training input data $\mathcal{D}$: $p(\mathcal{D}|\boldsymbol{\theta})$. There exist two main approaches in modeling with DNNs: discriminative and generative.

The discriminative approach implies parameterizing a conditional distribution over target values y: $p(y|\mathbf{x}, \boldsymbol{\theta})$. The training of DNNs allows identifying optimum parameters $\boldsymbol{\theta}^*$ based on a stochastic first-order optimization algorithm. In the case of classification tasks, the common choice for $p(y|\mathbf{x}, \boldsymbol{\theta})$ is a categorical distribution, in the case of regression - a Gaussian distribution (quite often with a constant variance). As it has been recently discovered: such models tend to be over-confident in their predictions with OoD inputs [Nguyen et al., 2015, Hendrycks and Gimpel, 2016]. This discovery may not be very surprising since MLE results in a point estimate and doesn't account for epistemic uncertainty. Taking into consideration the fact that in modern DNNs $|\boldsymbol{\theta}| \gg |\mathcal{D}|$, there may be several models $\boldsymbol{\theta}^*$ that generated $\mathcal{D}$.

Epistemic uncertainty can be estimated by inferring a posterior distribution: $p(\boldsymbol{\theta}|\mathcal{D})$ which can be done within the *Bayesian* frame of reference. Recently there were several promising results achieved with the discriminative DNNs for OoD detection utilizing *Bayesian* inference over model parameters [Blundell et al., 2015, Chen et al., 2014, Maddox et al., 2019].

The generative approach, on the other hand, allows learning the approximation of a true distribution over the training data: $p(\mathbf{x})$. The parameterization of this density is again done by DNNs, hence the name: deep generative models (DGMs). Since DGMs provide a mechanism to estimate the probability of a particular input then they should supposedly assign a low density to the OoDs. However, recent research revealed that such estimations are prone to errors as well and that DGMs often provide higher density values to OoDs than to in-distribution data [Nalisnick et al., 2018].

As it was the case with the discriminative deep models, to overcome this problem, one may use a *Bayesian* DGM that infers the posterior: $p(\boldsymbol{\theta}|\mathcal{D})$ for the training data $\mathcal{D}$ over the model parameters $\boldsymbol{\theta}$. Such an approach allows getting an ensemble of the approximations of a true distribution of the data where each sample from the posterior $\boldsymbol{\theta} \sim p(\boldsymbol{\theta}|\mathcal{D})$ gives a separate instance of the model in the ensemble. Based on sampling from the posterior distribution, it is

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possible to estimate the density of the input instance $p(\mathbf{x})$ taking into consideration epistemic uncertainty.

In this work, we implement several methods that are widely applicable to the *Bayesian* inference over DNN parameters, namely: Bayes by backpropagation (BBB) [Blundell et al., 2015], stochastic gradient Hamiltonian Monte-Carlo (SGHMC) [Chen et al., 2014], and Stochastic Weight Averaging-Gaussian (SWAG) [Maddox et al., 2019]. Most of the methods till now have been only applied to the discriminative supervised DNNs. It should be noted that despite the fact that theoretical justification for *Bayesian* VAEs was already present in the original paper [Kingma and Welling, 2013] (see Appendix F), there are still very few works addressing this point. In fact, to the best of our knowledge: there is only one paper dedicated to the BVAEs and OoD detection where only one of the methods (SGHMC) was used Daxberger and Hernández-Lobato [2019]. Our work represents an attempt to close this gap that is currently present between the discriminative and generative approaches based on DNNs. We transfer all of the mentioned methods to the deep generative VAEs and test them against several benchmarks suggested for OoD detection on various image datasets. Finally, based on our experiments we introduce a couple of simple scores for the OoD detection that surpass all baseline scores.

In short, we make the following main contributions:

- It is the first implementation of three different *Bayesian* approaches for VAEs estimating epistemic uncertainty.
- We do a practical benchmarking of the most frequently used scores for OoD detection taking into consideration *Bayesian* inference over the parameters of the likelihood of VAE.
- We suggest and apply two simple and efficient scores for the OoD detection that outperform baseline scores.
- We empirically evaluate the suggested approach based on several datasets.[1]

2 BACKGROUND

2.1 OUT-OF-DISTRIBUTION

Deploying a successful model requires the system to detect input data that are statistically anomalous or significantly different from those used during training. This is especially important for DNNs since they tend to produce overconfident predictions for such out-of-distribution (OoD) inputs [Lee et al., 2018]. The lack of reliability of supervised discriminative models based on DNNs, when faced with OoD, was recently addressed by various methods [Hendrycks and Gimpel, 2016, Hendrycks et al., 2018, Liang et al., 2017].

Unsupervised DGMs such as autoregressive models [van den Oord et al., 2016], Generative Adversarial Networks (GANs) [Goodfellow et al., 2014], flow-based models [Dinh et al., 2017, Kingma et al., 2017, Kingma and Dhariwal, 2018], and Variational Autoencoders (VAEs) [Kingma and Welling, 2013, Rezende et al., 2014] provide the opportunity to learn the density of the input data.

We choose to apply VAE as a particular instance of DGM in our experiments for several reasons:

1. It allows to obtain a particular value for the density in contrast to GANs that can only be sampled in a black-box manner.
2. It represents a model based on the latent variable, which seems like a reasonable assumption considering the complexity of the data's underlying density. The latent space has a much lower dimensionality in comparison with the dimensionality of the input. Such a bottleneck allows learning the most relevant features. It distinguishes VAE from the flow-based models where all the transformations are invertible and represent a bijective mapping between the input and the latent space [Dinh et al., 2017, Kingma and Dhariwal, 2018, Nielsen et al., 2020].
3. It allows the parametrization of all the *Bayesian* inference constituents, including the posterior over latent variable and the likelihood of the data [Kingma and Welling, 2013, Rezende et al., 2014]. Such separation of the constituents makes it possible to work with the particular part, as in our case, with the decoder of the VAE for weight uncertainty estimation, which distinguishes VAEs from the autoregressive models.

Furthermore, as it has been shown by Nalisnick et al. [2019], different DGM models may not produce similar results, which suggests that it is a good idea to concentrate only on one type for the analysis, which is represented by VAEs in our case.

However, it has been recently discovered that even in the case of DGMs that allows estimating the density, it does not work as intended and that DGMs return higher $p(\mathbf{x})$ for input data from a different distribution [Nalisnick et al., 2018].

There are several approaches to tackle this issue. One possible solution is to enhance the training dataset. Hendrycks et al. [2018] suggested incorporating the pre-selected anomalous examples employing the so-called outlier exposure technique, which achieved promising results. Ren et al. [2019] proposed a different method: two DGMs are trained separately—one for the semantics of the images and an-

[1] The source code for the results reproducibility is available at `https://github.com/xxxx/xxxx`

other for the background of the same images. The background images are generated with a substantial amount of noise to make the model learn this background discarding the image's semantics. Then by calculating the likelihood ratios between the model that learned semantics and the model that learned the background, it is possible to detect OoD. However, both of the suggested approaches rely on the knowledge of either the outlier or the background of the image, which cannot be reasonably covered for all the possible inputs. Moreover, recent research reveals that the likelihood ratio method does not achieve satisfactory results when *a Bayesian* VAE is applied [Daxberger and Hernández-Lobato, 2019]. Due to these reasons, we do not consider methods of dataset enhancement in this work.

Another possible solution is to devise an alternative score for the OoD detection. In that vein, the *Watanabe-Akaike Information Criterion* (WAIC) was successfully used by Choi et al. [2019]. Further, the disagreement score [Daxberger and Hernández-Lobato, 2019] was suggested for the same purpose. This idea was motivated within the information-theoretic framework and was also based on the posterior estimation over the model parameters. In both works, the considered scores were calculated based on the densities obtained from several models. In the former case, an ensemble was trained to calculate WAIC, while in the latter case, the *Bayesian* VAE was used. In addition, Nalisnick et al. [2019] introduced a typicality test of the input sequences under the conjecture that the inlier sequences should be members of the DGM's typical set.

We chose to address the OoD problem similarly: i.e., we suggest and apply new simple scores that help to detect OoDs.

2.2 VARIATIONAL AUTOENCODER

VAE represents a type of DGM that provides the possibility of density estimation of the input $\mathbf{x}$. The optimization objective of VAE is the evidence lower bound (ELBO), which allows joint optimization with respect to both variational parameters $\boldsymbol{\phi}$ of the encoder responsible for the variational approximation of the posterior $q_{\boldsymbol{\phi}}$ over the latent variable $\mathbf{z}$, and the generation parameters $\boldsymbol{\theta}$ of the decoder responsible for the parametrization of the likelihood of the input $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$:

$$\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x}) = E_{q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})}[\log p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}) - \log q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})] \tag{1}$$

VAEs are trained in an unsupervised manner from data and are widely used for generative purposes.

2.3 ESTIMATION OF THE MARGINAL LIKELIHOOD

Marginal likelihood can be computed in the following way:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) = \int_{\mathbf{z}} p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})p(\mathbf{z})d\mathbf{z} \tag{2}$$

However, it is difficult to calculate it precisely due to the integration over the whole $\mathbf{z}$-space. As suggested by Rezende et al. [2014], as soon as the VAE is trained, it is possible to estimate the marginal likelihood of the input under the generative model using *importance sampling* w.r.t to the approximated posterior, namely:

$$p_{\boldsymbol{\theta}}(\mathbf{x}) \simeq \frac{1}{N}\sum_{i=1}^{N}\frac{p_{\boldsymbol{\theta}}(\mathbf{x},\mathbf{z}_{(i)})}{q_{\boldsymbol{\phi}}(\mathbf{z}_{(i)}|\mathbf{x})}, \quad \text{where} \quad \mathbf{z}_{(i)} \sim q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) \tag{3}$$

However, as it has been discovered by Nalisnick et al. [2018], we cannot rely directly on the marginal likelihood estimations produced by a single DGM. As it was mentioned before, this fact is not surprising for the discriminative models based on DNNs. It should not be shocking for DGMs either taking into consideration that they are also based on the DNNs and that they also obtain the optimal parameters $\boldsymbol{\theta}^*$ under the maximum likelihood estimation (MLE) for the $p(\mathcal{D}|\boldsymbol{\theta})$ which represents a point estimate. Hence, without *Bayesian* inference over model parameters, it is impossible to estimate the epistemic uncertainty, which results in the model's inability to provide a robust estimation of the marginal likelihood for OoD inputs.

2.4 EPISTEMIC UNCERTAINTY

The required posterior estimation over model parameters $p(\boldsymbol{\theta}|\mathcal{D})$ in case of discriminative DNNs are usually implemented in the following three ways:

1. By using variational posterior approximation [Blundell et al., 2015];
2. By sampling from Markov Chain Monte Carlo [Chen et al., 2014];
3. By capturing the local geometry of the posterior through fitting a Gaussian with two first moments of the *Stochastic Gradient Descent* (SGD) [Maddox et al., 2019].

The first method represents a similar variational inference approach as in the case of VAEs when their encoders are trained to infer the posterior over the latent variable. The difference is that now it is applied to minimize the KL-divergence between the intractable posterior *over the model parameters* $p(\boldsymbol{\theta}|\mathcal{D})$ and the distribution from the family of tractable distributions $q(\boldsymbol{\theta}|\mathcal{D})$. It is also implemented by maximizing the ELBO. Since in our work we implement it in VAE, it means that we are making the variational inference for both the posterior for the latent variable conditioned on the input and the posterior for the parameters

conditioned on the training data. Such an approach is called fully *Bayesian* in the case of VAEs [Kingma and Welling, 2013]. There are various methods for approximating the posterior for the model parameters; we will use the one suggested in [Blundell et al., 2015].

Markov Chain Monte Carlo (MCMC) constructs a Markov chain with the desired posterior as its equilibrium distribution. The most known method for MCMC is based on the Metropolis-Hastings algorithm [Hastings, 1970, Metropolis and Ulam, 1949]. This algorithm converges to the real posterior by exploiting the random walk proposal distribution. However, this convergence may be pretty slow due to the slow exploration of the state space based on the random walk. *Hamiltonian Monte Carlo* (HMC) [Neal, 2012] postulates the exploration within the framework of the Hamiltonian dynamics. It allows producing distant proposals for the Metropolis algorithm resulting in much faster convergence. We use a variant of HMC adopted for deep learning, namely *Stochastic Gradient Hamiltonian Monte-Carlo* (SGHMC) that relies on the noisy gradient estimates [Chen et al., 2014].

Finally, it is possible to infer the desired posterior while training due to the noise in the SGD [Mandt et al., 2018]. We apply the *Stochastic Weight Averaging* (SWA) [Izmailov et al., 2019] together with fitting a Gaussian using the SWA solution as the first moment and covariance that is also derived from the SGD steps: the so-called SWAG method [Maddox et al., 2019]. SWAG is easy to implement since it does not require additional sampling and can be used as a baseline for the rest of the methods.

3 METHODOLOGY

3.1 BAYESIAN VAES

We implement several possible methods for *Bayesian* VAEs (BVAEs). We apply the *Bayesian* inference over the model parameters of the decoder of the VAE. Such a method allows sampling several decoders to form an ensemble with the subsequent marginal log-likelihood estimation as indicated in Equation 3. When the considered *Bayesian* epistemic uncertainty method requires a density function, we substitute it by its approximation, i.e., by ELBO.

Bayes by Backpropagation. We approximate the posterior distribution of the VAE decoder parameters given the training data $p(\boldsymbol{\theta}|\mathcal{D})$ based on the method suggested by Blundell et al. [2015]. This method was initially applied to discriminative learning. In our work, we implement it in VAEs. The ELBO objective is to find distribution parameters $\boldsymbol{\lambda}$ that minimize KL-divergence between our approximation and the true posterior; hence, the ELBO is formulated in the following way:

$$\mathcal{F}_{\boldsymbol{\theta}}(\mathcal{D}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\boldsymbol{\theta}|\boldsymbol{\lambda})}\Big[\log p(\mathcal{D}|\boldsymbol{\theta}) + \log p(\boldsymbol{\theta}) - \log q(\boldsymbol{\theta}|\boldsymbol{\lambda})\Big] \quad (4)$$

$\log p(\mathcal{D}|\boldsymbol{\theta})$ represents the sum of the marginal likelihoods of the individual inputs:

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{i=1}^{N} \log p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) \quad (5)$$

and

$$\log p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) \geq \mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x}^{(i)}) \quad (6)$$

where $\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x})$ is the ELBO for the marginal likelihood marginalized over the latent variable and it is defined in Equation 1. Since ELBO is the lower bound of the marginal likelihood, we can use it for our approximation. The optimization objective is formulated as:

$$\widetilde{\mathcal{F}_{\boldsymbol{\theta}}}(\mathcal{D}, \boldsymbol{\lambda}) = \mathbb{E}_{q(\boldsymbol{\theta}|\boldsymbol{\lambda})}\Big[\sum_{i=1}^{N}\Big[\mathcal{L}_{\boldsymbol{\theta},\boldsymbol{\phi}}(\mathbf{x}^{(i)})\Big] + \log p(\boldsymbol{\theta}) - \log q(\boldsymbol{\theta}|\boldsymbol{\lambda})\Big] \quad (7)$$

Now, if we plug in the right-hand side of the objective in Equation 1 we can get the Monte-Carlo estimation of the combined variational objective:

$$\widehat{\mathcal{F}_{\boldsymbol{\theta},\boldsymbol{\phi}}}(\mathcal{D}, \boldsymbol{\lambda}) \simeq \frac{1}{L}\sum_{j=1}^{L}\Big[\sum_{i=1}^{N}\Big[\log p_{\theta^{(j)}}(\mathbf{x}^{(i)}, \mathbf{z}) - \log q_{\phi}(\mathbf{z}|\mathbf{x}^{(i)})\Big] + \log p(\boldsymbol{\theta}^{(j)}) - \log q(\boldsymbol{\theta}^{(j)}|\boldsymbol{\lambda})\Big] \quad (8)$$

where $\boldsymbol{\theta}^{(j)}$ is sampled from the posterior $q(\boldsymbol{\theta}|\boldsymbol{\lambda})$, $\boldsymbol{z}$ is sampled from the posterior $q(\boldsymbol{z}|\boldsymbol{x})$ and N is taken equal to the batch size.

For the minimization objective, we use the negated estimate: $-\widehat{\mathcal{F}_{\boldsymbol{\theta},\boldsymbol{\phi}}}(\mathcal{D}, \boldsymbol{\lambda})$. We assume a diagonal Gaussian distribution for both variational posteriors with parameters μ and σ. In order to make σ be always non-negative we apply the same reparametrization as it was suggested by Blundell et al. [2015], namely $\sigma = \log(1+\exp(\rho))$, yielding the following posterior parameters $\lambda = (\mu, \rho)$. For the prior over the latent variable, we use the standard normal density, for the prior over the weights we use the scale mixture of two Gaussians as in [Blundell et al., 2015].

The usual reparametrization trick [Kingma and Welling, 2013] is applied to both $\boldsymbol{\theta}$ and $\boldsymbol{z}$ for training by backpropagation.

Stochastic Gradient Hamiltonian Monte Carlo. This approach exploits sampling instead of optimization, which was the case with BBB. This sampling is done within the *Markov Chain Monte Carlo* (MCMC) framework, and it is based on the proposals generated utilizing the Hamiltonian dynamics. Namely, assume that the posterior distribution:

$$p(\boldsymbol{\theta}|\mathcal{D}) \propto \exp(-U(\boldsymbol{\theta}, \mathcal{D})) \tag{9}$$

where $U(\boldsymbol{\theta}, \mathcal{D})$ stands for the potential energy function in the Hamiltonian.

In our work, we take:

$$U(\boldsymbol{\theta}, \mathcal{D}) = -\log p(\boldsymbol{\theta}, \mathcal{D}) = -\sum_{i=1}^{N} \log p(\mathbf{x}^{(i)}|\boldsymbol{\theta}) - \log p(\boldsymbol{\theta}) \tag{10}$$

where $\log p(\mathbf{x}^{(i)}|\boldsymbol{\theta})$ is approximated by ELBO in our experiments and $\log p(\boldsymbol{\theta})$ is the prior over parameters.

Since *Hamiltonian Monte Carlo* (HMC) requires the computation of the gradient for the whole batch, a stochastic gradient alternative has been suggested by Chen et al. [2014] which relies on the noisy gradients and allows proposal generation in a faster mini-batch manner.

In our work, we also apply the improvements suggested by Springenberg et al. [2016] which significantly reduce the number of hyperparameters by means of adaptive estimates of the parameters in question during the burn-in procedure and subsequent training. Such an approach has been previously implemented in the unsupervised generative setting with VAEs by Daxberger and Hernández-Lobato [2019].

Stochastic Weighted Averaging-Gaussian. SWAG is fitting the following Gaussian distribution:

$$\mathcal{N}\left(\theta_{\text{SWA}}, \widehat{\Sigma_{\text{SWA}}}\right) \tag{11}$$

where θ_{SWA} is a running average over DNN parameters and Σ_{SWA} is the sample covariance matrix that after T epochs can be calculated as:

$$\theta_{\text{SWA}} = \frac{1}{T}\sum_{i=1}^{T}\theta_i \quad \text{and} \quad \Sigma_{\text{SWA}} = \frac{1}{T-1}\sum_{i=1}^{T}\left(\theta_i - \theta_{\text{SWA}}\right)\left(\theta_i - \theta_{\text{SWA}}\right)^{\top} \tag{12}$$

Since Σ_{SWA} is of a very high rank it is approximated by the K last epochs during training resulting in $\widehat{\Sigma_{\text{SWA}}}$[Maddox et al., 2019].

SWAG was previously applied only to the discriminative DNNs, in our work we implement it within a generative approach with VAEs.

Combining several likelihoods. After the approximation of the variational posterior over the weights, the usual practice is to estimate the expected likelihood, the exact form of which can be formulated as follows:

$$p(\mathbf{x}^*|\mathcal{D}) = \int p(\mathbf{x}|\theta)p(\theta|\mathcal{D})d\theta \tag{13}$$

The unbiased estimate of which can be obtained like this:

$$\mathbb{E}_{p(\theta|\mathcal{D})}[p(\mathbf{x}^*|\theta)] \simeq \frac{1}{N}\sum_{i=1}^{N} p(\mathbf{x}|\theta_i); \quad \text{where} \quad \theta \sim p(\theta|\mathcal{D}) \tag{14}$$

$p(\mathbf{x}|\theta_i)$ is computed by importance sampling as in Eq. 3. As soon as the expected likelihood is estimated, one can apply a threshold that would distinguish if the considered input adheres to the in-distribution sample or not.

In [Choi et al., 2019] the likelihoods returned by several generative models are used to estimate the *Watanabe Akaike Information Criterion* (WAIC):

$$WAIC(\mathbf{x}^*|\mathcal{D}) = \mathbb{E}_{p(\theta|\mathcal{D})}[p(\mathbf{x}|\theta)] - Var_{p(\theta|\mathcal{D})}[p(\mathbf{x}|\theta)] \tag{15}$$

WAIC estimates the gap between the expected likelihood and the variance between the obtained likelihoods, which should benefit the small variance cases.

Another alternative is to calculate the disagreement score $D[\cdot]$ suggested by Daxberger and Hernández-Lobato [2019]. This score measures the variation in the likelihoods $\{p(\mathbf{x}^*|\boldsymbol{\theta}_i)_{i=1}^{N}\}$ which captures the uncertainty of the models within the ensemble about the particular input:

$$D_{\Theta}[\mathbf{x}^*] = \frac{1}{\sum_{\theta\in\Theta} w_\theta^2}; \quad \text{where} \quad w_\theta = \frac{p(\mathbf{x}^*|\boldsymbol{\theta})}{\sum_{\theta\in\Theta} p(\mathbf{x}^*|\boldsymbol{\theta})} \tag{16}$$

The lower the score, the more informative the input is about the parameters $\boldsymbol{\theta}$, and, consequently, the uncertainty value is higher.

The weights represent the normalized likelihoods between 0 and 1. The disagreement score sums up the squares of the weights and takes the reciprocal. If the score is large, it means that all models return close values of the likelihoods. On the contrary, if the score is 1, then there is one model that dominates.

Finally, Nalisnick et al. conjectured that due to the high dimensionality of inputs the reason for the over-confidence of DGMs may be due to the fact that in-distribution images lie in the typical set in contrast to the tested OoDs that concentrate in the high-density region. Based on this conjecture, they introduced the test for typicality that treats all input sequences of length M as inliers if their entropy is sufficiently close to the entropy of the model, i.e., if the following holds for small ϵ then the given M-sequence is in-distribution:

$$\left| \frac{1}{M} \sum_{m=1}^{M} -\log p\left(\mathbf{x}_m; \boldsymbol{\theta}\right) - \mathbb{H}[p(\mathbf{x}; \boldsymbol{\theta})] \right| \leq \epsilon \tag{17}$$

We applied this score to one-element sequences since it is the most realistic scenario in practical applications of OoD detection.

Our scores. Based on the results of the experiments with the available metrics on all of the considered methods, we decided to apply our scores that capture the variation. In our work, we apply two simple scores for the same purpose. First, we measure the information entropy of the normalized likelihoods, namely:

$$\mathbb{H}_{\Theta}[\mathbf{x}^*] = -\sum_{\theta \in \Theta} w_\theta \log w_\theta; \quad \text{where} \quad w_\theta = \frac{p(\mathbf{x}^*|\boldsymbol{\theta})}{\sum_{\theta \in \Theta} p(\mathbf{x}^*|\boldsymbol{\theta})} \tag{18}$$

It is a standard information-theoretic metric that measures the average information of the distribution: the lower the entropy, the more one of the models is confident about the predicted value. The entropy measure is applied to the normalized likelihoods. Such normalization may be considered as the categorical distribution over the obtained marginal likelihoods of the models.

Secondly, we calculate the sample standard deviation of the marginal log-likelihoods returned by the models within the ensemble:

$$\Sigma_{\Theta}[\mathbf{x}^*] = \sqrt{\frac{1}{N-1} \sum_{\theta \in \Theta} (\log p(\mathbf{x}^*|\boldsymbol{\theta}) - \overline{\log p(\mathbf{x}^*|\boldsymbol{\theta})})^2} \tag{19}$$

It measures the variation within the log-likelihoods directly without normalizing step as in the case of the entropy, so if the variation persists along with the considered methods and datasets, the standard deviation will capture this difference: the higher the value, the more uncertainty there is between the models about a particular input.

Thresholding. There is also an open question of the appropriate threshold selection for the model evaluation. We tackle this problem in the same way as Hendrycks and Gimpel [2016] by applying threshold-independent metrics (i.e., metrics that are calculated for all possible thresholds) such as the *Area Under the Receiver Operating Characteristic Curve* (AUROC), the *Area Under Precision-Recall curve* (AUPR), and the *False-Positive Rate at 80% of True-Positive Rate* (FPR80) [Davis and Goadrich, 2006].

4 EVALUATION

We run all of our experiments on the four image datasets: MNIST [LeCun and Cortes, 2010], Fashion-MNIST [Xiao et al., 2017], SVHN [Netzer et al., 2011], and CIFAR-10 [Krizhevsky et al., 2010]. As it has been observed in the past [Ren et al., 2019, Nalisnick et al., 2018], the likelihood estimations may be misled by the dataset they have been trained on. For instance, if the model has been trained on MNIST and OoD detection has been performed on the Fashion-MNIST, then the researcher, only by chance, may obtain good results. To avoid such mistakes, we train our models on all the datasets and check the following in-distribution vs. OoD: MNIST vs. Fashion-MNIST and vice versa, SVHN vs. CIFAR-10, and vice versa.

First, we estimate the impact of the latent space's number of dimensions on the loss function. The dimensionality is closely connected with the dataset the model is trained on. MNIST and FashionMNIST results reveal no need to go over ten latent dimensions since loss function did not significantly decrease after that value. For SVHN and CIFAR-10, we experimented with the number of latent dimensions up to 100; the most optimal results have been achieved with dimensionality equals 20 for SVHN and 70 for CIFAR-10.

We experimented with two different architectures for all of our tests: one for the grayscale images and the second one for the RGB images with 1 and 3 channels correspondingly. All models have been trained for 1000 epochs. For the evaluation of the inputs, we sampled 200 different models for our ensemble and evaluated them on a separate test data split of 5120 images that models have not been trained on.

For our implementation of Bayes by backpropagation, we noticed that random Normal initializer of the DNNs weights suggested as a prior in the original paper Blundell et al. [2015] resulted in very slow convergence. To speed up the process, we also experimented with the following parameters: random Normal initializer with 0 mean and 0.1 standard deviations for μ and constant initializer for $\rho = -3$, which improved the training speed [2] Krishnan and Esposito [2020].

In case of SGHMC we adhere to the same protocol as in Daxberger and Hernández-Lobato [2019], namely, we use the same scale-adapted sampler [3] implementation with learning rate 10^{-3} for the training and momentum decay 0.05. We also place Gaussian priors over decoder parameters with precision $p(\theta) = \mathcal{N}(0, \lambda^{-1})$ and with Gamma hyperprior over the precision $p(\lambda) = \Gamma(\alpha, \beta)$ with $\alpha = \beta = 1$ that are resampled on each epoch.

For the experiments with SWAG, we set $K = 40$ and kept the default values for all the rest hyperparameters as in the original SWAG implementation.[4]

[2] For BBB we used the PyTorch *Bayesian* layers available at `https://github.com/IntelLabs/bayesian-torch`

[3] SGHMC sampler that we used is available at `https://github.com/automl/pybnn`

[4] SWAG sampler that we used is available at `https://github.com/wjmaddox/swa_gaussian`

Table 1: Scoring values across all types of *Bayesian* VAEs trained on Fashion-MNIST data and tested on MNIST as OoD

	Fashion-MNIST vs. MNIST								
	BBB			**SGHMC**			**SWAG**		
	ROC AUC↑	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**
Expected LL	40.43	45.46	95.20	40.43	45.18	94.99	25.09	38.01	99.54
WAIC	59.53	59.35	71.88	55.79	53.86	74.56	19.90	35.14	99.83
Typicality test	40.51	43.40	86.36	41.02	43.85	86.05	56.40	50.32	64.88
Disagreement score	96.44	97.22	1.11	95.25	96.31	2.50	79.98	80.74	38.24
Entropy (ours)	97.97	98.43	**0.19**	97.28	97.92	**0.53**	**82.50**	**84.05**	**35.61**
Stds of LLs (ours)	**99.64**	**99.55**	0.34	**99.56**	**99.50**	0.55	19.90	34.22	94.42

Table 2: Scoring values across all types of *Bayesian* VAEs trained on CIFAR-10 data and tested on SVHN as OoD

	CIFAR-10 vs. SVHN								
	BBB			**SGHMC**			**SWAG**		
	ROC AUC↑	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**
Expected LL	59.73	53.27	58.99	60.39	53.74	58.08	60.31	53.51	57.05
WAIC	61.15	54.22	57.15	62.39	55.38	55.07	64.29	55.81	50.59
Typicality test	63.73	60.89	65.53	64.44	61.05	64.01	64.93	61.52	64.33
Disagreement score	81.16	84.82	38.47	80.41	83.00	40.61	73.27	76.95	54.95
Entropy (ours)	84.76	**88.21**	29.31	84.56	86.90	29.12	**76.51**	**80.54**	49.37
Stds of LLs (ours)	**89.98**	85.83	**16.03**	**92.52**	**91.48**	**12.27**	71.26	64.65	**44.34**

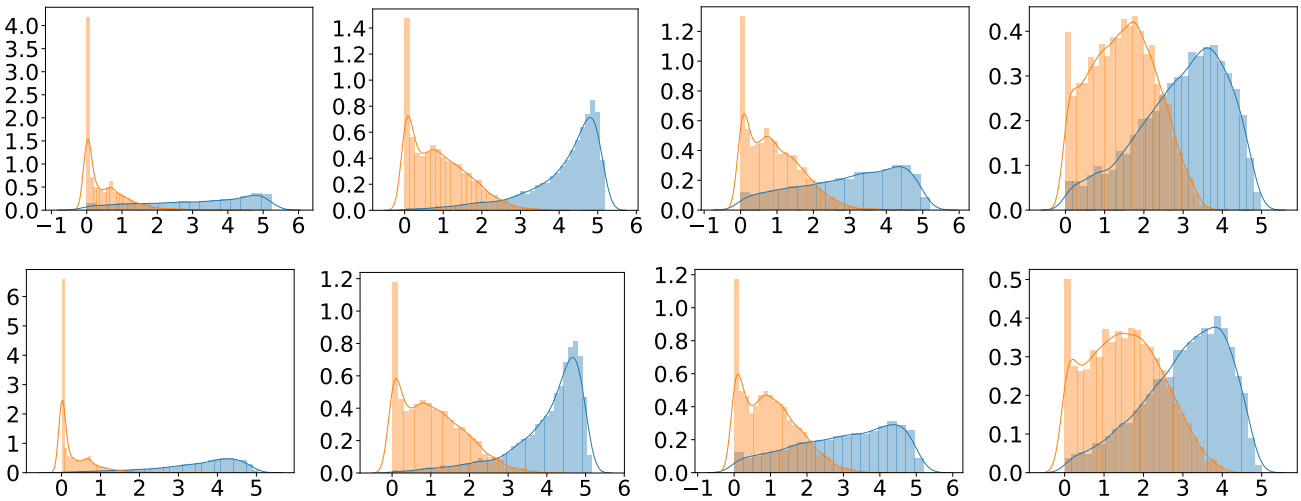

Figure 1: Histograms of the entropies of the marginal likelihoods. LLs are estimated based on sampling from the *Bayesian* VAEs, blue depicts in-distribution (ID) and orange: out-of-distribution (OoD). **From left to right**: MNIST as ID vs Fashion-MNIST as OoD, Fashion-MNIST as ID vs MNIST as OoD, SVHN as ID vs CIFAR-10 as Ood, CIFAR-10 as ID vs SVHN as OoD. **Top:** Sampling is done from Bayes-by-backprop VAE. **Bottom:** Sampling is done from SGHMC VAE.

All the experiments are done within the framework implemented by Nielsen et al. [2020].

The results of the experiments for all datasets and models can be observed in the Tables 1 - 4. As it can be seen, *Bayesian* methods used in the discriminative approach can be successfully applied also for the generative models such as VAEs for OoD detection. Moreover, it can be observed that the variation among the model densities persists across all of the types of the *Bayesian* VAEs and all the datasets. The best results are achieved for BBB and SGHMC types of VAEs. The simple entropy score consistently demonstrates state-of-the-art results while detecting OoD by better capturing the variation in comparison with the previously introduced baseline scores, the histograms for both BBB and SGHMC VAE results are shown in Figure 1. The sample standard deviation significantly outperforms the entropy score in the case of BBB and SGHMC methods.

Table 3: Scoring values across all types of *Bayesian* VAEs trained on MNIST data and tested on Fashion-MNIST as OoD

	MNIST vs. Fashion-MNIST								
	BBB			**SGHMC**			**SWAG**		
	ROC AUC↑	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**
Expected LL	99.98	99.98	0.00	99.93	99.92	0.04	**96.83**	**96.20**	**5.18**
WAIC	99.99	99.99	0.00	**99.94**	**99.94**	0.02	80.37	76.25	33.56
Typicality test	99.98	99.98	0.00	99.88	99.90	0.00	94.91	96.47	1.58
Disagreement score	98.95	99.01	0.23	97.32	97.70	1.37	94.88	93.97	8.99
Entropy (ours)	99.42	99.47	0.02	98.50	98.75	0.29	95.72	95.20	8.37
Stds of LLs (ours)	**99.99**	**99.99**	**0.00***	99.91	99.91	**0.00***	80.37	82.78	39.12

* 0's are possible since it is a value for false-positive rate at 80% of true-positive rate

Table 4: Scoring values across all types of *Bayesian* VAEs trained on SVHN data and tested on CIFAR-10 as OoD

	SVHN vs. CIFAR-10								
	BBB			**SGHMC**			**SWAG**		
	ROC AUC↑	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**	**ROC AUC↑**	**AUPRC↑**	**FPR80↓**
Expected LL	58.65	61.79	77.72	57.09	60.56	80.18	58.98	62.06	76.52
WAIC	64.46	66.01	68.39	62.17	64.38	72.45	62.84	68.42	75.25
Typicality test	44.63	44.28	81.46	43.35	43.63	82.45	44.28	44.13	81.96
Disagreement score	85.20	88.35	30.26	85.31	88.52	28.66	77.58	80.36	45.60
Entropy (ours)	87.80	90.63	20.77	87.89	90.76	19.91	**80.01**	**83.24**	**41.58**
Stds of LLs (ours)	**93.29**	**91.51**	**10.99**	**94.70**	**93.95**	**8.67**	59.31	53.36	61.78

5 CONCLUSION

In this paper, we implemented three different methods for estimation of epistemic uncertainty in the generative setting based on VAEs utilizing *Bayesian* inference over model parameters: BBB based on variational inference, SGHMC based on Monte-Carlo sampling, and SWAG based on the noise in the SGD. We tested them against the frequently used OoD benchmarks: expected log-likelihood, WAIC, disagreement score, and typicality test. We observed that both BBB and SGHMC demonstrated comparable performance. While SWAG was always lagging behind in comparison with other methods, we conclude that it can still be used as a simple baseline for epistemic uncertainty also in the case of VAEs in the same manner as in the case of the discriminative approach. Moreover, during our experiments, we noticed that the most promising score was based on the idea of the variation of marginal likelihoods. Built on that, we proposed using two simple scores: one is based on the information entropy and the second - on the standard deviation for the robust unsupervised OoD detection. With them, we achieved state-of-the-art results across all the benchmarked methods and all the considered datasets. Future work may be revolved around a deeper understanding of the significance of the variation for the OoD detection.

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