Bayesian OOD detection with aleatoric uncertainty and outlier exposure

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Abstract

Typical Bayesian approaches to OOD detection use epistemic uncertainty. Surprisingly from the Bayesian perspective, there are a number of methods that successfully use aleatoric uncertainty to detect OOD points (e.g. Hendryks et al. 2018). In addition, it is difficult to use outlier exposure to improve a Bayesian OOD detection model, as it is not clear whether it is possible or desirable to increase posterior (epistemic) uncertainty at outlier points. We show that a generative model of data curation provides a principled account of aleatoric uncertainty for OOD detection. In particular, aleatoric uncertainty signals a specific type of OOD point: one without a well-defined class-label, and our model of data curation gives a likelihood for these points, giving us a mechanism for conditioning on outlier points and thus performing principled Bayesian outlier exposure. Our principled Bayesian approach, combining aleatoric and epistemic uncertainty with outlier exposure performs better than methods using aleatoric or epistemic alone.

1 Introduction

The most typical approach to Bayesian OOD distribution detection uses epistemic uncertainty (Lakshminarayanan et al. 2017; Malinin & Gales 2018; Malinin et al. 2020; Wen et al. 2019; Choi et al. 2018; Postels et al. 2020), while other work implicitly combines aleatoric and epistemic uncertainty by looking at the overall predictive entropy (Izmailov et al. 2021; Ovadia et al. 2019; Maddox et al. 2019). Surprisingly from the Bayesian perspective, there are a large number of methods that successfully use aleatoric uncertainty alone to detect OOD points (Malinin & Gales 2018; Liu et al. 2018; Hendrycks & Gimpel 2016; Jiang et al. 2017; Lee et al. 2017; Liu et al. 2018; Hendrycks et al. 2018). In addition, many of these methods can be trained on OOD points, in a process known as outlier exposure (OE).

When suitable OOD data is available, OE leads to dramatic increases in performance (Hendrycks et al. 2018). However, developing a principled Bayesian method using OE is difficult. In particular, a principled Bayesian formulation would involve treating the OE points as providing extra terms in the likelihood. However, it not currently clear how to create a likelihood for outlier points. Instead, current OE methods use a variety intuitively reasonable objectives, which have no interpretation as log-likelihoods and thus cannot be combined with Bayesian inference.

In this paper, we provide a principled account of how to incorporate aleatoric uncertainty and outlier exposure into Bayesian OOD detection methods. In particular, we consider a model of the curation process...
applied during the original creation of datasets such as CIFAR-10 and ImageNet. Critically, this curation process is designed to filter out a specific set of OOD points: those without a well-defined class label. For simplicity, we will refer to these points as OOD for the remainder of the paper. For instance, if we try to classify an image of a radio as cat vs dog, there is no well-defined class label, and we should not include that image in the training set. We model curation as a consensus-formation process. In particular, we give each image to multiple human annotators: if the image has a well-defined label (Fig. 1 left and middle), they will all agree, consensus will be reached and the datapoint will be included in the dataset. In contrast, if the human annotators are given an image with an undefined class label (Fig. 1 right), all they can do is to choose randomly, in which case they disagree, consensus will not be reached and the datapoint will be excluded from the dataset. Critically, that random final choice corresponds to aleatoric, not epistemic uncertainty. If we ask a human to classify an image of a radio as cat vs dog, the issue certainly is not that the human annotator is uncertain about the radio’s degree of “cat-ness” or “dog-ness”. The issue is that we are forcing the human to answer a fundamentally nonsensical question, and the only reasonable response is to choose randomly. That random choice thus corresponds to aleatoric uncertainty, and thus aleatoric uncertainty can signal that the point is OOD, and has an undefined class label. Our model gives a likelihood for being OOD (or having an “undefined class label”) in terms of the underlying classifier probabilities, allowing us to incorporate outliers in principled Bayesian inference. We find that our approach, incorporating OE and aleatoric uncertainty with Bayes performs better than a standard Bayesian approach without OE, and better than a standard aleatoric uncertainty based approach with OE (e.g. [Hendrycks et al. 2018]).

2 Background

In the introduction, we briefly noted that different annotators will agree about the class label when that class label is well-defined, but will disagree for OOD inputs without a well-defined class label (if only because they are forced to the label the image and the only thing they can do is to choose randomly). Interestingly, a simplified generative model which considers the probability of disagreement amongst multiple annotators has already been developed to describe the process of data curation [Aitchison 2020 2021]. In data curation, the goal is to exclude any OOD images to obtain a high-quality dataset containing images with well-defined and unambiguous class labels. Standard benchmark datasets in image classification have indeed been carefully curated. For instance, in CIFAR-10, graduate student annotators were instructed that “It’s worse to include one that shouldn’t be included than to exclude one”, then [Krizhevsky et al. 2009] “personally verified every label submitted by the annotators”. Similarly, when ImageNet was created, [Deng et al. 2009] made sure that a number of Amazon Mechanical Turk (AMT) annotators agreed upon the class before including an image in the dataset.

[Aitchison 2021] proposes a generative model of data curation that we will connect to the problem of OOD detection. Given a random input, \( X \), drawn from \( P(X) \), a group of \( S \) annotators (indexed by \( s \in \{1, \ldots, S\} \)) are asked to assign labels \( Y_s \in \mathcal{Y} \) to \( X \), where \( \mathcal{Y} = \{1, \ldots, C\} \) represents the label set of \( C \) classes. If \( X \) is OOD, annotators are instructed to label the image randomly. We assume that if the class label is well-defined, sufficiently expert annotators will all agree on the label, so consensus is reached, \( Y_1 = Y_2 = \cdots = Y_S \), and the image will be included in the dataset. Any disagreement is assumed to arise because the image is OOD, and such images are excluded from the dataset. In short, the final label \( Y \) is chosen to be \( Y_1 \) if consensus was reached and \( \text{Undef} \) otherwise (Fig. 1B).

\[
Y|\{Y_s\}_{s=1}^S = \begin{cases} 
Y_1 & \text{if } Y_1 = Y_2 = \cdots = Y_S \\
\text{Undef} & \text{otherwise} 
\end{cases}
\]

From the equation above, we see that \( Y \in \mathcal{Y} \cup \{\text{Undef}\} \), that is, \( Y \) could be any element from the label set \( \mathcal{Y} \) if annotators come to agreement or \( \text{Undef} \) if consensus is not reached. Suppose further that all annotators are IID (in the sense that their probability distribution over labels given an input image is the same). Then,
Figure 2: An example of the generative model of dataset curation, with $S = 3$. Three annotators are instructed to classify images as cats or dogs. The left and middle images have well-defined class-labels as they are clearly a cat and a dog respectively. Therefore, the annotators all give the same answer and consensus is reached. However, the right-most image is OOD (it has an undefined class label), so the annotators are forced to give random answers; they disagree and we remove the image from the dataset.

Figure 3: Graphical models under consideration. A The generative model for standard supervised learning with no data curation. B The generative model with data curation. (Adapted with permission from Aitchison, 2021).

The probability of $Y \in \mathcal{Y}$ can be written as

$$P (Y = y | X, \theta) = P \left( \{Y_s = y\}_{s=1}^S | X, \theta \right) = \prod_{s=1}^S P (Y_s = y | X, \theta) = P (Y_s = y | X, \theta)^S = p^S_y (X)$$

(2)

where we have abbreviated the single-annotator probability as $p_y (X) = P (Y_s = y | X, \theta)$. When consensus is not reached (no consensus), we have:

$$P (Y = \text{Undef} | X, \theta) = 1 - \sum_{y \in \mathcal{Y}} P (Y = y | X, \theta)$$

$$= 1 - \sum_{y \in \mathcal{Y}} p^S_y (X).$$

(3)

Notice that the maximum of Eq. (3) is achieved when the predictive distribution is uniform: $p_y = 1/C, \forall y \in \mathcal{Y},$ as can be shown using a Lagrange multiplier $\gamma$ to capture the normalization constraint,

$$L = \left( 1 - \sum_y p^S_y \right) + \gamma \left( 1 - \sum_y p_y \right)$$

$$= \frac{\partial L}{\partial p_y} = -Sp^S_y - \gamma$$

(4)

(5)

The value of $p_y$ with maximal $L$ is independent of $y$, so $p_y$ is the same for all $y \in \mathcal{Y}$, and we must therefore have $p_y = 1/C$. In addition, the minimum of zero is achieved when one of the $C$ classes has a probability

$p_y (X) = 1$. Therefore, an input with high predictive (aleatoric) uncertainty is, by definition, an input with a high probability of disagreement amongst multiple annotators, which corresponds to being OOD.

3 Methods

We are able to form a principled log-likelihood objective by combining Eq. (2) for inputs with a well-defined class-label (denoted by $D_{in}$) and Eq. (3) for OOD inputs without a well-defined class label (denoted by $D_{out}$). However, this model was initially developed for cold-posteriors (Aitchison, 2021) and semi-supervised learning (Aitchison, 2020) where the no-consensus inputs were not known and were omitted from the dataset. In contrast, and following Hendrycks et al. (2018), we use proxy datasets for OOD inputs, and explicitly maximize the probability of inputs from those proxy datasets having being OOD (Eq. [8]). Importantly, now that we explicitly fit the probability of an undefined class-label, we need to introduce a little more flexibility into the model. In particular, a key issue with the current model is that more annotators, $S$, implies a higher chance of disagreement hence implying more OOD images. Thus,
arbitrary choices about the relative amount of training data with well-defined and undefined class-labels might cause issues. To avoid any such issues, we modify the undefined-class probability by including a base-rate or bias parameter, \( c \), which modifies the log-odds for well-defined vs undefined class-labels. In particular, we define the logits to be,

\[
\ell_0 = c + \log \left(1 - \sum_{y \in Y} p_y^S(X)\right)
\]

\[
\ell_{y \in Y} = \log p_y^S(X)
\]

(6)

(7)

where \( p_y(X) \) is the single-annotator probability output by the neural network.

\[
P(Y = \text{Undef} | X, \theta) = \frac{e^{\ell_0}}{e^{\ell_0} + \sum_{y \in Y} e^{\ell_y}}
\]

\[
P(Y = y | X, \theta) = \frac{e^{\ell_y}}{e^{\ell_0} + \sum_{y \in Y} e^{\ell_y}}
\]

(8)

(9)

with \( c = 0 \), this reverts to Eq. (2) and (3), while non-zero \( c \) allows us to modify the ratio of well-defined to undefined class-labels to match that in the training data.

Of course, we do not have the actual datapoints that were rejected during the data curation process, so instead \( D_{\text{out}} \) is a proxy dataset (e.g. taking CIFAR-10 as \( D_{\text{in}} \), we might use downsampled ImageNet with 1000 classes as \( D_{\text{out}} \)). The objective is,

\[
\mathcal{L} = \mathbb{E}_{D_{\text{in}}} [\log P(Y = y | X, \theta)] + \lambda \mathbb{E}_{D_{\text{out}}} [\log P(Y = \text{Undef} | X, \theta)]
\]

(10)

where \( \lambda \) represents the relative quantity of inputs with undefined to well-defined class-labels. We use \( \lambda = 1 \) both for simplicity and because the inclusion of the bias parameter, \( c \), should account for any mismatch between the “true” and proxy ratios of inputs with well-defined and undefined class-labels. In addition, we use a fixed value of \( S = 10 \) as is suggested by [Aitchison (2021)] and we learn \( c \) via backpropagation during training.

Lastly, since our objective is a well-defined likelihood function that jointly models \( D_{\text{in}} \) and \( D_{\text{out}} \), we can easily turn our model into a fully Bayesian one by adding a prior distribution on the neural network parameters, \( \theta \), and then perform approximate inference approaches (e.g. stochastic gradient Markov chain Monte Carlo) to estimate the posterior distribution over \( \theta \). The use of Bayesian inference in our approach allows us to incorporate both epistemic uncertainty and aleatoric uncertainty when detecting OOD samples and we will show in next section that combining two types of uncertainty together can lead to performance superior than using either of them alone.

4 Results

4.1 Toy data

First, we conducted an experiment on a toy dataset. We use the make_moons generator from Scikit-learn ([Pedregosa et al., 2011]) to generate labelled examples of two classes, with 2000 examples per class (Fig. 4 and 5). For synthetic OOD points, we use 2000 samples generated from the make_circles generator (Fig. 5).

We trained a three-layer fully connected neural network with 32 hidden units in each hidden layer for 20 epochs using Adam ([Kingma & Ba, 2015]) with a constant learning rate of \( 5 \times 10^{-3} \). Initially, we trained without data with undefined class-labels (Fig. 4), and plotted the OOD probability, \( P(Y = \text{Undef} | X, \theta) \), with high undefined probabilities and uncertain classifications being denoted by darker colors. This classifier is very certain for all inputs, and therefore judges there to be a well-defined class-label almost everywhere, except in a small region around the decision boundary. In contrast, when training with OOD inputs (Fig. 5), the model learns to take points around the training data as having a well-defined class-label (lighter colors), then classifies points further away as being OOD (darker colors).

4.2 Image classification

In this section, we demonstrate the effectiveness of our approach via large scale image classification experiments. We considered two different baselines, in addition to our method. First, in “BNN”, we followed the usual OOD detection procedure for Bayesian neural networks in training on our in-distribution dataset, \( D_{\text{in}} \), using SGLD, and ignored our OOD dataset, \( D_{\text{out}} \), as it is not clear how to incorporate these points into a classical Bayesian neural network. Second, in “OE”, we used the non-Bayesian method of [Hendrycks et al. (2018)], which trains on \( D_{\text{in}} \), and incorporates an objective that encourages uncertainty on \( D_{\text{out}} \). Our method uses a BNN, as in the BNN baseline, but additionally trains on \( D_{\text{out}} \) using the log-likelihood from Eq. (3) to increase uncertainty on those points.

Datasets We used CIFAR-10 and CIFAR-100 as \( D_{\text{in}} \), and downsampled ImageNet as our training \( D_{\text{out}} \). The Downsampled ImageNet dataset introduced by [Oord et al. (2016)] is a downsampled version of ImageNet ([Deng et al., 2009a]) with the labels removed. The dataset is designed for unsupervised learning tasks such as density estimation and image generation.

\[\text{access governed agreement at } \text{image-net.org/download.php} \text{, underlying images are not owned by ImageNet and have a mixture of licenses}\]
At test time, we consider a number of OOD datasets that the model was not trained on, as proposed in Hendrycks & Gimpel (2016) and as implemented by Hendrycks et al. (2018):

1. Isotropic zero-mean Gaussian noise with $\sigma = 0.5$
2. Rademacher noise where each dimension is $-1$ or $1$ with equal probability.
3. Blobs data of algorithmically generated amorphous shapes with definite edges
4. Texture data (Cimpoi et al., 2014) of textural images in the wild.
5. SVHN (Netzer et al., 2011) which contains 32x32 colour images of house numbers.

**OOD score** At test time, to distinguish between OOD and in-distribution examples, we need a score that measures the model’s uncertainty. There are several model-specific choices. In our model one can choose to use the OOD probability (Eq. 3) as the score. Hendrycks & Gimpel (2016); Hendrycks et al. (2018) use the negative maximum softmax probability (Hendrycks & Gimpel, 2016). However, to ensure a fair comparison, we used one metric that makes sense for all methods considered, the total uncertainty (Depeweg et al., 2018). The total uncertainty is the entropy of the predictive distribution, marginalising over uncertainty in the neural network parameters, $\mathcal{H}(p(y \mid x^*))$, which equals the sum of aleatoric uncertainty and epistemic uncertainty. Note that the total uncertainty from OE only contains aleatoric uncertainty since the model is fully deterministic. In contrast, the standard BNN and our BNN approach both have aleatoric and epistemic uncertainty. The key differences is that in our model, the aleatoric uncertainty is shaped by outlier exposure, whereas in a standard BNN, the aleatoric uncertainty is determined solely by the in-distribution data.

**Evaluation metrics** OOD detection is in essence a binary classification problem.

It is therefore sensible to use metrics for binary classification to evaluate a model’s ability to detect OOD inputs. As such, to allow for comparison to past work we use two metrics. First, the area under the receiver operating characteristic curve (AUROC) indicates how well the model can discriminate between positive and negative classes, for example, a model with AUROC of 0.9 would assign a higher probability to an input with undefined class-label than one with a well-defined class-label 90% of the time. A perfect model would have an AUROC of 1.0 while an uninformative model with random outputs would have an AUROC of 0.5.

Secondly, the false positive rate at $N\%$ true positive rate (FPR) computes the probability of an input being misclassified as having an undefined class-label (false positive) when at least $N\%$ of the true inputs with undefined class-labels are correctly detected (true positive). In practice, we would like to have a model with low FPR since an ideal model should detect nearly all inputs with undefined class-labels while raising as few false alarms as possible. In our experiments, we let $N = 95$.

**Networks and training protocols** As is mentioned above, our experiments involve comparison among outlier exposure (OE), Bayesian neural network (BNN) and our proposed approach (Ours).

The network architecture is chosen to be a 40-2 Wide Residual Network (Zagoruyko & Komodakis, 2016) for all experiments. OE was trained directly using the
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| Dataset | $D_{in}$ | $D_{test}$ | AUROC $\uparrow$ | FPR95 $\downarrow$ |
|---------|---------|----------|------------|------------|
| Gaussian | 91.73±8.88 | 94.99±3.80 | 100.00±0.0 | 13.91±11.05 | 9.03±5.83 | 0.00±0.0 |
| Rad. | 93.78±3.90 | 95.96±1.70 | 100.00±0.0 | 11.01±7.05 | 7.62±2.49 | 0.00±0.0 |
| CIFAR-10 | Blob | 89.41±2.44 | 90.57±2.38 | 100.00±0.0 | 35.16±5.19 | 33.25±10.17 | 0.00±0.0 |
| Textura | 89.39±0.49 | 88.21±1.16 | 95.25±0.63 | 37.61±1.14 | 52.17±6.15 | 25.19±3.93 |
| SVHN | 90.42±1.83 | 93.33±0.89 | 97.27±0.52 | 28.55±4.36 | 19.43±2.46 | 12.28±2.28 |
| CIFAR-100 | Blob | 93.16±3.38 | 80.10±8.97 | 100.00±0.0 | 14.47±5.45 | 32.92±12.43 | 0.00±0.0 |
| Rad. | 85.39±6.51 | 95.34±5.69 | 100.00±0.0 | 26.60±11.01 | 10.95±8.35 | 0.00±0.0 |
| SVHN | 75.97±0.52 | 75.15±1.05 | 85.07±0.47 | 69.74±2.27 | 76.72±2.74 | 58.43±2.09 |
| Texture | 81.04±0.73 | 77.85±2.20 | 89.66±1.77 | 52.18±2.90 | 63.67±6.24 | 42.70±5.57 |

Table 1: Experimental results on a range of different datasets for AUROC and FPR95. Note the arrows indicate the “better” direction (e.g. so higher AUROC is better). $D_{in}$ represents the in-distribution dataset. $D_{test}$ is the testing out-of-distribution dataset. (The results reported are mean and standard error computed over 6 runs of different random seeds.)

For BNN and our approach, we used Cyclical Stochastic Gradient MCMC (Zhang et al., 2020) to perform approximate inference over the network parameters. The implementation and learning rate scheduling largely followed Zhang et al. (2020). In particular, the cycle length was chosen to be 50 epochs and we ran 4 cycles in total. At each cycle, we stored weights at the last epoch and we ran 4 cycles in total. At each cycle, we stored weights at the last 3 epochs as samples from the approximate posterior. In addition, we used a temperature of 0.1 on the likelihood for the baseline BNN, so as to match $S = 10$ in the labelled likelihood for our model (Eq. 2 Aitchison 2020). For all experiments, at each iteration, we feed the network with a mini-batch made up of 128 samples from $D_{in}$ and 256 samples from $D_{out}$ such that $D_{out}$ will not usually be entirely traversed during a training epoch.

**Results** Broadly, we found that our approach gave superior performance to the OE and BNN using AUROC and FPR95 (Table 1).

## 5 Related work

The most closely related prior work is that on OOD detection using epistemic uncertainty. The history of this idea is a bit difficult to trace, as the idea evolved rapidly into benchmark for Bayesian neural networks (Lakshminarayanan et al., 2017 Louizos & Welling 2017, Pawlowski et al., 2017 Krueger et al., 2017 Henning et al., 2018 Maddox et al., 2019 Ovadia et al., 2019 Fortuin et al., 2021), with very few papers written directly about OOD detection using BNNs (though see Malinin & Gales, 2018).

At the same time, a variety of approaches based on aleatoric uncertainty were developed. This line of work started with Hendrycks & Gimpel (2016), who used the maximum softmax probability for a pre-trained network to identify OOD points. Better separation between in and out of distribution points was obtained by Liang et al. (2017) by temperature scaling and perturbing the inputs, and Probably Approximately Correct (PAC) guarantees were obtained by Liu et al. (2018). Later work trained on OOD data using an objective such as the cross entropy to the uniform distribution (Lee et al., 2017 Hendrycks et al., 2018 Dhamija et al., 2018). The requisite OOD data was either explicitly provided (Hendrycks et al., 2018) or obtained using a generative model (Lee et al., 2017). In contrast, our method provides a formal account of aleatoric uncertainty based OOD detection as maximizing a likelihood, and integrates it with Bayesian epistemic uncertainty.

Compared with utilising a model’s predictive uncertainty, a perhaps more straightforward approach is to train a binary classifier to perform OOD detection. The required OOD inputs can be obtained from a proxy OOD dataset (DeVries & Taylor 2018 Hendrycks et al., 2018), by taking misclassified points to be OOD (DeVries & Taylor 2018), or can be generated from a generative model (Vernek et al., 2019 Guénaïs et al., 2020). However, approaches based on predictive uncertainty are generally found to perform better than those based on explicitly classifying OOD points (Hendrycks et al., 2018). This might be expected as classification based approaches rely on the presence of an OOD dataset, whereas approaches based on predictive uncertainty (Hendrycks & Gimpel, 2016) are able to extract useful information even in the absence of an outlier dataset.
There is also work on “classification with rejection”, in high-risk settings such as medical decision making, where there is a very high cost for misclassifying an image (e.g., failing to diagnose cancer could lead to death). As such, the machine learning system should defer to a human expert whenever it is uncertain (perhaps because the model capacity is limited, it has not seen enough data, or the medical expert has side-information) (e.g. [Herbei & Wegkamp, 2006, Bartlett & Wegkamp, 2008, Cortes et al., 2016, Mozannar & Sontag, 2020]). Importantly, in classification with rejection there is a well-defined right answer for the rejected inputs, and we defer to the human expert because it is critically important to get that right answer. In contrast, in our setting, there is no meaningful right answer for the rejected inputs: (e.g. classify an image of a radio as cat vs dog). Therefore, an expert would not be able to classify our rejected points because the corresponding ground-truth class-label is fundamentally ill-defined, and if forced to make a classification, all they could do is to choose a random label.

Finally, it is possible to solve the OOD detection task by fitting a generative model of inputs, and declaring inputs with low probability under that model as OOD [Wang et al., 2017, Pidhorskyi et al., 2018]. However, there are considerable subtleties in getting this approach to work well [Nalisnick et al., 2018, Choi et al., 2018, Shafaei et al., 2018, Hendrycks et al., 2018, Ren et al., 2019, Morningstar et al., 2020], as having a high probability under the probabilistic generative model does not necessarily mean than an input point is typical of the dataset. The generative approach is often much more difficult to apply in practice, simply due to the much greater difficulty in training good generative models, as compared with training classifiers.

6 Conclusion

We developed a likelihood for UCL points (a subset of OOD points), and used it to integrate OE methods within principled Bayesian inference. The resulting Bayesian OE method gave superior performance to other methods, including pure aleatoric uncertainty and Bayesian methods without OE.

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