Improve Uncertainty Estimation for Unknown Classes in Bayesian Neural Networks with Semi-Supervised / One Set Classification

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Abstract

Although deep neural network (DNN) has achieved many state-of-the-art results, estimating the uncertainty presented in the DNN model and the data is a challenging task. Problems related to uncertainty such as classifying unknown classes (class which does not appear in the training data) as known class with high confidence, is critically concerned in the safety domain area (e.g., autonomous driving, medical diagnosis). In this paper, we show that applying current Bayesian Neural Network (BNN) techniques alone does not effectively capture the uncertainty. To tackle this problem, we introduce a simple way to improve the BNN by using one class classification (in this paper, we use the term “set classification” instead). We empirically show the result of our method on an experiment which involves three datasets: MNIST, notMNIST and FMNIST.

1 Introduction

In many fields, especially computer vision and natural language processing, DNN have achieved many state-of-the-art results on tasks such as image recognition [KSH12] [HZRS16], segmentation [HGDG17], machine translation [VSP+17], etc. Estimating the uncertainty presented in DNN model is important for critical task [KG17]. One principle way to measure the uncertainty or confidence of the prediction is based on the statistic such as predictive mean, entropy and variance, using Bayesian machine learning, i.e. BNN if our model is a DNN[Nea12]. Beside capturing the parameters uncertainty, other methods works with modifying the loss function [DT18], [KG17], by which the model attempts to learn the heteroscedastic aleatoric uncertainty, i.e. uncertainty that depends on the input data (e.g. if there is an occlusion on the image object, our model will less likely to produce accurate prediction so we train our model such that it recognize "occlusion").

Experiments in previous paper [RBB18], [LPB17], the estimated predictive posterior is used to detect out-of-distribution data, or data from unknown class by measuring the its statistics. In other words, they expect data from unknown class to have high entropy and variance by using BNN. In this paper, we show that Bayesian learning in general can only capture partial uncertainty of the model. In classification tasks, the machine learning model cannot effectively detect data from unknown classes because we have implicitly conditioned that there is a limit number of labels in our future data. We introduce a simple method, which is inspired from unsupervised learning, to help the DNN model effectively capture data from unknown classes by questioning whether the data is in the known label or not. It should be noted that as we are trying to discriminate between unknown and known classes, we use the term "set classification" to avoid confusion. We, however, do not deny the effectiveness of Bayesian learning, indeed, we experimentally show that we can get the best of both worlds by combining them together.

2 Background

2.1 Bayesian Neural Networks

Given a training dataset $D_N = \{(x_i, o_i)\}_{i=1}^N$ for which $x_i$ is an $i^{th}$ input and $o_i$ is the $i^{th}$ output. In a classification task, our parameterized classifier models the probability $p(o|x, \theta, D)$ where $\theta$ is parameters in our model. In DNN, these parameters are learned by using backpropagation...
algorithm [RHW85], minimizing a predefined loss function, e.g. cross entropy with regularization. In Bayesian machine learning, given a test data point $o^*, x^*$ we wish to capture the posterior $p(o^*|x^*, D)$.

$$p(o^*|x^*, D) = \int p(o^*|x^*, \theta)p(\theta|D)d\theta$$  \hspace{1cm} (1)

The term $p(\theta|D)$ is a posterior of weight:

$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$  \hspace{1cm} (2)

Both Eq.1 and Eq.2 are computationally intractable in the case of DNN. In fact, they are intractable even for the case of simple classification model such as logistic regression [Bis]. The general approach to approximate Eq.2 is to define parameterized variational distribution $q_\omega(\theta)$ that minimize the Kullback–Leibler divergence: $KL(q_\omega(\theta), p(\theta|D))$ [LPB17] [GG16]. [KW13]. The predictive poster is approximated by Monte Carlo (MC) sampling on the variational distribution instead of original distribution. In this paper, we adopt the idea of MC dropout [GG16] for the experiment.

To show that Bayesian inference do not fully capture the uncertainty, consider a 2D toy example in Fig.1. We build our model to classify two known classes, 'cat' and 'dog'. The blue line our learned maximum a posterior (MAP) solution with cross validation. The pink region illustrates the uncertainty region of our model from Bayesian learning. During test time, we feed into the input 'cow' image. In this case, Bayesian learning is capable of detecting unknown classes based on the uncertainty measurement since the 'cow' images cluster lies near the uncertainty region. On the other hand, even though the 'chicken' images cluster location is far from the training distribution, the model still classifies 'chicken' images with high confidence.

2.2 Set Classification

Determined whether a label of given data is familiar or unknown relates to the problem of one class classification or anomaly detection. Methods such as One-class SVM, One-class neural network [MY01], [MY07] are able to effectively detects outlier on documents data. For DNN trained on image data, [RR17] introduces a simple idea of using an autoencoder for detecting novel image while works such as [LLLS17] exploit the characteristic of Generative Adversarial Neural (GAN) network for detecting the outlier. In the case of one set classification, we are only given data which belong to our set. Thus, it often requires prior knowledge to determine the probability of whether the given the data is belonged to our set or not. Absolute probability (either zero or one) would likely to give us overconfident estimation. We will explain in details the interpretation of this probability in sec.3.2.

In this paper, we adopt the idea of using autoencoder as a memory for estimating the probability in the semi-supervised manner, i.e. making use of unlabeled data. In the case of image data, we first train our autoencoder on both labeled and unlabeled data, minimizing the reconstruction error. After this, we use encoded layer to train a set classifier based on the limited negative labeled data, which means that the data belonged to unknown class. By this way, we are less bias towards our sentiment about the data distribution. Furthermore, the user can have a good reference to tune the probability according to their prior knowledge or desire like industry requirement. As stated previous, the disadvantage of this method is that we need to label some amount of negative data to train the model.
3 Combined Approach

3.1 Posterior Predictive Distribution

In classification problem, each $o_i$ is labeled as one of the value in set $C = \{c_m\}_{m=1}^K$. In many real scenarios, such as image recognition, each input value $x_j$ can be classified as $y_j$ which is not in the set $C$. We denote $C^*$ as a complement set of $C$ i.e., $C^*$ contains data whose labels are not in $C$, and $\bar{c}$ is a class which indicates that the data is in $C^*$. The output $y_j$ in this case, can take one value either in set $C$ or $\bar{c}$. By this way, we can calculate the probability $p(y|x)$ as follows:

$$p(y|x) = \sum_{s \in \{C, C^*\}} p(y, s|x) = \sum_{s \in \{C, C^*\}} p(y|s, x)p(s|x)$$

$$= p(y|s = C, x)p(s = C|x) + p(y|s = C^*, x)p(s = C^*|x) \quad (3)$$

The posterior probability $p(y|s = C, x)$ from (3) can be estimated with Bayesian learning from training dataset $D_N$. In the case our model is a DNN, we can estimate this posterior by using existing methods introduced in section 2.1 such as MC Dropout [GG16], Laplace approximation [RBB18], SGLD [WT11] and setting $p(y = \bar{c}|s = C, x)$ to 0 since this is conditioned that the data is in the set $C$. On the other hand, the posterior probability $p(y|s = C^*, x)$ is computed by setting $p(y = \bar{c}|s = C^*, x) = 1$ and other $c_m \in C$ to 0. In this paper, the term $p(s|x)$ is estimated based on methods in section 2.2. It is possible to inference $p(s|x)$ with Bayesian learning by using MC dropout as well. In this work, maximum likelihood is used as an approximation for posterior distribution $p(s|x)$, we estimate the mean of the posterior $p(y|x)$ as follow:

$$\mathbb{E}[p(y = d_i|x)] \approx \widehat{\mathbb{E}}[p(y = d_i|x)] = p(s = C^*|x) + \frac{1}{T}p(s = C|x) \sum_i^T p(y = d_i|\theta_i, s = C, x) \quad (4)$$

where $\theta_i \sim q_\omega(\theta), d_i \in C \cup \{\bar{c}\}$ for $i = 1, 2, ..., K+1$.

Beside allowing the model to decide whether the input data is in known class or not, we also use predictive entropy [Sha48] to measure the uncertainty.

$$H(y|x) := - \sum_{i}^{K+1} p(y = d_i|x) \log p(y = d_i|x)$$

$$\approx - \sum_{i}^{K+1} \widehat{\mathbb{E}}[p(y = d_i|x)] \log \widehat{\mathbb{E}}[p(y = d_i|x)] \quad (5)$$

In the next sub-section, we show the interpretation from both predictive entropy and posterior mean output of our model.

3.2 Uncertainty Interpretation

As discussed previously, unlike other Bayesian Deep Learning works, which prevent the model to give overconfident output for anomaly input by summarizing based on the uncertainty estimation from posterior of each samples such as predictive entropy, disagreement score [LPB17], the output from our method is more conservative since we include the additional unknown class $\bar{c}$. In this section, we show how to interpret the uncertainty using our approach. We consider these possible cases:

- $p(y = \bar{c}|x) > 0.5$, the model detect that the data as unknown classes with high confidence

- $p(y = \bar{c}|x) < 0.5$ and $\arg \max_{d_i} p(y|x) = \bar{c}$ (e.g., $[p_{\text{cat}}, P_{\text{dog}}, P_{\text{ele}}] = [0.32, 0.28, 0.4]$ in the cat, dog example, our input is a ”cow” which possesses a face like a dog and legs like a cat), the data has features that often appear in the training set but there is a presence of unfamiliar features which is strong enough to make our model decide that the data is unknown.

- $p(y = \bar{c}|x) < 0.5$, $\arg \max_{d_i} p(y|x) = c_m$ with high predictive entropy $H(y|x)$ (e.g., $[p_{\text{cat}}, P_{\text{dog}}, P_{\text{ele}}] = [0.45, 0.15, 0.4]$), similar to the second case, the only difference is that there are many features in the data the resemblance in training set. Even though $p(y = c_m|s = C, x) = 0.75$, $p(s|x)$ has penalized the confidence of the model.

3
- $p(y = \bar{c}|x) < 0.5$, \( \arg \max_d p(y|x) = c_m \) with high predictive entropy \( H(y|s = C, x) \) and the model is confident that the data is a known classes since most of the features appear in training data (e.g., \([p_{cat}, p_{dog}, p_e] = [0.49, 0.47, 0.04]\)). The input lies near the decision boundary of the manifold \( p(y|s = C, x) \).

- \( \arg \max_d p(y|x) = c_m \) with low predictive entropy \( H(y|x) \), the model is confident of its prediction that the data is in known class with high certainty.

If our one class classification outputs either 1 or 0 for every input, then the decision system has become overconfident for its measurement, since in the second and third cases above will be depends solely on our in-class classifier. Final note is that since our model also adopt the idea of BNN, with the expressive power of DNN, data in known class which are misclassified should have a high predictive entropy.

4 Experiments

We use three datasets in this experiments: MNIST, notMNIST and FMNIST with details in Table 1. Assume that we only have limited labeled data in notMNIST dataset to train our set classifier. We first train a deep convolutional autoencoder (DCA) from MNIST training data, and notMNIST data (both labeled and unlabeled) with the architecture as follow: input[28x28], convolutional filters (Conv)[32x3x3, Relu], max pooling (MaxPool)[2x2], Conv[64x3x3, Relu], MaxPool[2x2] (encoded layer), Conv[64x3x3, tanh], up sampling[2x2], Conv[32x3x3, relu], up sampling[2x2], Conv[1x3x3, sigmoid]. From this DCA, we train a MNIST classifier \( p(y|s = C, x) \) from the encoded layer with a fully hidden connected layer of size 128 (dropout rate = 0.5), followed by a softmax output layer with dropout rate = 0.25. We train our set classifier \( p(s|x) \) by connecting encoded layer with a 256x64 densely connected layers followed by a softmax output layer with dropout rate = 0.25. The predictive posterior mean and entropy on MNIST and FMNIST test set are estimated from (Eq. 4) and (Eq. 5) with \( T = 100 \).

Fig. 2 shows the histogram of misclassified data on FMNIST dataset (classifying unknown classes as known class). We shown candidate images in Fig.3, it should be noted that the shape of reconstructed image resembling the original image, and they have some features of the digit they were misclassified into. From section 3.2, we would expect that the accuracy on FMNIST dataset from our approach when using MC dropout (Bayesian Learning) and without MC dropout is roughly the same (Table 1) since the set classifiers for these two case are similar. To show the effectiveness of BNN over regularly DNN, we plot a distribution estimated from histogram of predictive mean entropy of the misclassified data on FMNIST dataset in Fig. 4a. Clearly, BNN

|                         |                |
|-------------------------|----------------|
| MNIST Training data     | 55000          |
| MNIST Validation data   | 5000           |
| MNIST Testing data      | 10000          |
| notMNIST labeled data   | 4000           |
| notMNIST unlabeled data | 10000          |
| FMNIST testing data     | 10000          |
| Accuracy on MNIST Testing data (MC dropout) | 0.9116 |
| Accuracy on MNIST Testing data (no MC dropout) | 0.9116 |
| Accuracy on FMNIST Testing data (MC dropout) | 0.7045 |
| Accuracy on FMNIST Testing data (no MC dropout) | 0.7023 |

Table 1: Summary of dataset and results
results gives us a much more better uncertainty estimates, corresponding to higher entropy in this case. We also show how our method improve BNN approach by plotting the similar entropy distribution for the data our approach correctly classify as unknown class in Fig. 4b. By using set classification, our method have high confidence (low entropy) that the data is unknown, on the other hand, BNN with dropout still give high confidence prediction that the data is belong to familiar classes. Finally, we show the entropy distribution on MNIST test dataset and as we expected, data which are misclassified tends to have high uncertainty presented in the predictive posterior.

Figure 3: Example of FMNIST images which are misclassified as MNIST image by our approach. Each column contains a predicted class, original image and reconstructed image using our autoencoder. Shown images which are misclassified from 0 to 8, their associated mean value of predict posterior are larger than 0.8 (some images, such as the 4th images, has value as high as 0.91). For the image which is misclassified as number 9, the associated value is 0.7 (maximum value we found)

Figure 4: (a) Estimated distribution based on histogram of predictive entropy on FMNIST data which the two methods wrongly misclassified as known classes, both methods used set classification. (b) Estimated distribution based on histogram of predictive entropy on FMNIST data which our approach correctly classify as unknown class. We calculated the predictive entropy of BNN using MC dropout without set classification to show that there are many cases that can be detected using our approach while BNN cannot. (c) The same distribution for MNIST testing data using our approach. Although it is not shown here, BNN using MC dropout achieved similar result (in fact they overlap each other)

5 Conclusion

In this paper, we have shown the limitation of Bayesian Learning and how combining set classification and Bayesian Learning can improve the uncertainty estimate to data which belong to unknown class. However, it should be noted that our approach does not completely solve the problem of misclassifying unknown classes as known classes. To our knowledge, although no verification have yet been done, we suspect that the reason for the error is that our discriminator and autoencoder do not effectively learn the spatial relation of the known classes. We believe that it would be interesting to see how incorporating spatial relation by using method such as recurrent neural network [LH15] can improve the current situation.
For other possible future works, we would like to apply this approach for active learning scenario and for other computer vision tasks such as detection and segmentation. We also would like to improve our loss function to capture heteroscedastic aleatoric uncertainty.

References

[Bis] Christopher Bishop. Pattern recognition and machine learning.

[DT18] Terrance DeVries and Graham W Taylor. Learning confidence for out-of-distribution detection in neural networks. arXiv preprint arXiv:1802.04865, 2018.

[GG16] Yarin Gal and Zoubin Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In international conference on machine learning, pages 1050–1059, 2016.

[HGDG17] Kaiming He, Georgia Gkioxari, Piotr Dollár, and Ross Girshick. Mask r-cnn. In Computer Vision (ICCV), 2017 IEEE International Conference on, pages 2980–2988. IEEE, 2017.

[HZRS16] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 770–778, 2016.

[KG17] Alex Kendall and Yarin Gal. What uncertainties do we need in bayesian deep learning for computer vision? In Advances in Neural Information Processing Systems, pages 5580–5590, 2017.

[KSH12] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolutional neural networks. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 25, pages 1097–1105. Curran Associates, Inc., 2012.

[KW13] Diederik P Kingma and Max Welling. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114, 2013.

[LH15] Ming Liang and Xiaolin Hu. Recurrent convolutional neural network for object recognition. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 3367–3375, 2015.

[LLLS17] Kimin Lee, Honglak Lee, Kibok Lee, and Jinwoo Shin. Training confidence-calibrated classifiers for detecting out-of-distribution samples. arXiv preprint arXiv:1711.09325, 2017.

[LPB17] Balaji Lakshminarayanan, Alexander Pritzel, and Charles Blundell. Simple and scalable predictive uncertainty estimation using deep ensembles. In Advances in Neural Information Processing Systems, pages 6405–6416, 2017.

[MY01] Larry M Manevitz and Malik Yousef. One-class svms for document classification. Journal of machine Learning research, 2(Dec):139–154, 2001.

[MY07] Larry Manevitz and Malik Yousef. One-class document classification via neural networks. Neurocomputing, 70(7-9):1466–1481, 2007.

[Nea12] Radford M Neal. Bayesian learning for neural networks, volume 118. Springer Science & Business Media, 2012.

[RBB18] Hippolyt Ritter, Aleksandar Botev, and David Barber. A scalable laplace approximation for neural networks. In International Conference on Learning Representations, 2018.

[RHW85] David E Rumelhart, Geoffrey E Hinton, and Ronald J Williams. Learning internal representations by error propagation. Technical report, California Univ San Diego La Jolla Inst for Cognitive Science, 1985.
[RR17] Charles Richter and Nicholas Roy. Safe visual navigation via deep learning and novelty detection. In Proc. of the Robotics: Science and Systems Conference, 2017.

[Sha48] Claude Elwood Shannon. A mathematical theory of communication. Bell system technical journal, 27(3):379–423, 1948.

[VSP+17] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In Advances in Neural Information Processing Systems, pages 6000–6010, 2017.

[WT11] Max Welling and Yee W Teh. Bayesian learning via stochastic gradient langevin dynamics. In Proceedings of the 28th International Conference on Machine Learning (ICML-11), pages 681–688, 2011.