Deep Bayesian Neural Network Performance Measurement

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Abstract

Deep Bayesian neural network has aroused a great attention in recent years since it combines the benefits of deep neural network and probability theory. Because of this, the network can make predictions and quantify the uncertainty of the predictions at the same time, which is important in many life-threatening areas. However, most of the recent researches are mainly focusing on making the Bayesian neural network easier to train, and proposing methods to estimate the uncertainty. I notice there are very few works that properly discuss the ways to measure the performance of the Bayesian neural network. Although accuracy and average uncertainty are commonly used for now, they are too general to provide any insight information about the model. In this paper, we would like to introduce more specific criteria and propose several metrics to measure the model performance from different perspectives, which include model calibration measurement, data rejection ability and uncertainty divergence for samples from the same and different distributions.

1 Introduction

Deep neural network has been proved to be a very powerful tool in many applications, such as image processing and natural language processing. But a major drawback of neural network is the network could falsely give over-confident predictions [17], which is very likely to bias a person’s judgement in practice. This is dangerous in many life-threatening areas, for example, medicine. Due to this reason, researchers are now aware that giving a predictive distribution rather than a single point estimation is a more rational way since a distribution could describe the mean and variance at the same time, therefore, the uncertainty could be helpful to assist decision making process.

Bayesian neural network plays an important role in uncertainty estimation. It represents uncertainty by placing distributions over the model parameters, and the uncertainty is passed through the network when a sample is fed into it. Eventually, the uncertainty can be captured at the output layer [7]. There are several modern approaches to train the Bayesian neural network in order to get the posterior distribution for the inference. Markov Chain Monte Carlo (MCMC) was a standard procedure for inference with neural networks [7]. However, considering such method is too computational expensive, researchers prefer to approximate the posterior distribution through variational inference, which was brilliantly generalized by Kingma and Welling through reparameterization trick [11]. This work inspired people to bring in variational approximation into the entire network and Bayes by Backpropagation (BBB) provided an end-to-end solution for variational approximation in Bayesian neural network, the details can be found in [4]. After that, people tried to implement BBB on different architectures, for instance, CNN [8] and RNN [12]. In 2018, Google ensembles these methods into Bayesian layers to make variational inference as standard components in model design pipeline [9]. Instead of using BBB, Gal and Ghahramani proved that dropout can be treated as variational approximation [13][14], this approach dramatically decreases the number of trainable parameters in the network comparing to BBB, which seems like a more rational choice in practical applications.

those techniques mentioned above have greatly shaped the Bayesian deep learning research field. However, how to measure the performance of deep Bayesian neural networks and how to decide which model to be used under different scenarios are still lacking proper discussion and worth discovering. In this paper, we propose several approaches to measure the performance of a model from three different perspectives. the remainder of the paper is organized as follows: Section 2 discusses commonly used approaches to assess the performance of a network. Section 3 introduces three proposed perspectives for model assessment. Section 4 demonstrates these approaches on MNIST, Fashion-MNIST. Lenet and a very simple 2 layer feed-forward network are used during this process. We then have a brief conclusion in Section 5.

The contribution of this work are:

1 The code can be found at https://github.com/yikuanli/ModelPerformance
• Proposed three perspectives to estimate the performance of Deep Bayesian Neural Network
• Based empirical CDF of entropy, we proposed rejection ability metrics to estimate the ability of a model to reject samples from different distributions and accept samples follow the same distribution.
• Proposed the uncertainty and probability diagrams and the average uncertainty divergence to measure the prediction reliability of a model.

2 Common Bayesian Model Performance Measurement

The problem we look in this paper is supervised multi-class classification with Bayesian neural networks. Each sample has input \( x \in \chi \) and label \( y \in \gamma = \{1, 2, ..., K\} \). The training process is to learn the true posterior distribution given observed data \( D \). During inference, the predictive distribution is represented as below \[3\]:

\[
p(y^*|x^*, D) = \int_{\Omega} p(y^*|x^*) p(\omega|D) d\omega
\]

where \( x^* \) and \( y^* \) are new input and new output, and \( p(\omega|D) \) is posterior distribution. Considering the fact that the true posterior is intractable, this paper uses variational inference, which designs a variational distribution to approximate the true posterior distribution by optimizing the Evidence Lower Bound (ELBO). Then, Monte Carlo sampling is used to get an estimation of the variational predictive distribution \[6\]:

\[
q_\theta(y^*|x^*) = \frac{1}{T} \sum_{t=1}^{T} p(y^*|x^*, \hat{\omega}_t)
\]

where \( \hat{\omega}_t \) is weight that randomly drawn from variational distribution \( q_\theta(\omega) \).

2.1 Accuracy and Fusion Matrix

In classification task, accuracy and fusion matrix are most commonly used tools to estimate the model performance. Accuracy directly shows the ratio of samples that can be correctly classified in the dataset. And fusion matrix, which is normally represented as Receiver Operating Characteristic(ROC) curve and Precision-Recall(PR) curve, indicates the model ability to separate samples to different classes \[10\]. Most of the current researches on Bayesian neural network are mainly using accuracy, precision and recall as major criteria to compare model performance.

2.2 Model Uncertainty

The Bayesian deep neural network is well-known because it is capable of capturing the predictive uncertainty. This uncertainty includes the uncertainty comes from the data called aleatoric uncertainty and the uncertainty comes from the model called epistemic uncertainty \[17\]. Kendall and Gal decomposed the predictive uncertainty into these two uncertainties in \[1\] and Kwon and his colleagues improved the decomposition specifically for classification task \[6\], which is shown as below.

\[
alacor = \frac{1}{T} \sum_{t=1}^{T} \text{diag}(\hat{p}_t) \ast \hat{p}_t \ast \hat{p}_t \ast \hat{p}_t
\]

\[
epistemic = \frac{1}{T} \sum_{t=1}^{T} (\hat{p}_t - \bar{p}) \ast \bar{p} \ast \bar{p}
\]

where \( \bar{p} = \sum_{t=1}^{T} \hat{p}_t / T \), \( \hat{p}_t = p(\hat{\omega}_t) = \text{Softmax}(f^{\hat{\omega}_t}(x^*)) \), \( v \ast v = vv^T \).

Besides accuracy, precision and recall as standard tools to measure the performance of a deep neural network, currently, the most commonly used approach to compare the uncertainty performance of two Bayesian models is calculating the average aleatoric uncertainty and average epistemic uncertainty tested on dataset with the same distribution as the training dataset. Under this condition, we expect the model could give smaller uncertainty which indicates that model is more confident on the predictions, past works like \[8\] \[17\] \[6\] \[1\] \[2\] all used such metrics to compare performance of model uncertainty.
2.3 Model Calibration

Accuracy and average model uncertainty mentioned above are the most commonly used methods to measure Bayesian model performance. But researchers gradually start to pay attention to other aspects now. One of the most useful approaches is model calibration, the problem of predicting probability estimates representative of the true correctness likelihood. We can call it universal probability or true probability in classification task. Model calibration is important in many areas, for instance, medicine. A doctor usually expects the model provides a true probability for the prediction. If a model is poorly calibrated, the prediction could bias a doctor’s judgement and cause series problems. [5] [15] thoroughly discussed ways to measure the calibration performance. The details will be introduced in Section 3 in reliability diagram and expected calibration error.

3 Three perspectives to measure Bayesian Model

Besides using accuracy, ROC, PRC and average uncertainty. In this paper, we propose three different perspectives to measure the performance of Bayesian model.

3.1 Rejection Ability

Generally, in classification task, we expect a model is able to correctly predict a sample that comes from the same distribution with a high confidence score. In addition, we also expect a model is able to give each potential class a low confidence score when a sample is out of distribution. In this case, an engineer could setup a threshold to decide the type of sample to reject or accept by the model. [16] used empirical CDF over the range of possible entropies on out of distribution dataset to illustrate which model has better uncertainty estimates. Although empirical CDF of entropy is a useful visual tool, it is more convenient to have a scalar summary statistic of rejection ability. One notion of the rejection ability is the difference in model reject samples from different distribution and accept samples from the same distribution. Since probability does not like entropy, which has various range between 0 to infinite, we can use the area under the empirical CDF of probability to indicates the rejection ability. Obviously, for the samples from the same distribution as the training set, the area under the empirical CDF of probability curve (AUPC) should be small, and the AUPC for the samples from different distribution should be large. As a result, given two datasets, one with the same distribution as the training set and the other one with different distribution from the training set, the rejection ability for a model on these two dataset is defined as follows, the value is between 0 and 1 and larger value means better rejection ability, an example is shown in Figure 2:

\[ RA = AUC(AUPC(DD)) - AUC(AUPC(DS)) \] (5)

Where DD means samples from a different distribution and DS means samples from the same distribution, AUC represents area under the curve.

3.2 Calibration Error

As mentioned above, model calibration is important in many tasks. [5] illustrated that reliability diagrams and expected calibration error were excellent methods to measure the calibration error. The reliability diagrams are a visual representation of model calibration and expected calibration error gives a scalar value to indicate the performance.

3.2.1 Reliability Diagrams

The reliability diagrams relate the accuracy with confidence, saying accuracy is a function of confidence. If the model is well-calibrated, then the diagram is a identity function. Otherwise, a model has miscalibration. In order to estimate the function from finite samples, we separate samples into M groups based on their prediction confidence. Then calculate the accuracy within each group. If a model is perfectly calibrated, the accuracy of each group should match corresponding prediction confidence [5]. For instance, for samples with prediction
confidence within interval \( I_m = \left( \frac{m-1}{M}, \frac{m}{M} \right) \).

\[
\text{acc}(I_m) = \frac{1}{N_m} \sum_{i \in N_m} 1(\hat{y}_i = y_i)
\]

(6)

Where \( N_m \) is number of samples in group \( m \), \( \hat{y}_i \) and \( y_i \) are the predicted label and true label for sample \( i \).

The confidence for interval \( I_m \) is shown as follows:

\[
\text{conf}(I_m) = \frac{1}{N_m} \sum_{i \in N_m} \hat{p}_i
\]

(7)

Where \( \hat{p}_i \) is the confidence for sample \( i \). One thing worth noting here is that, in Bayesian inference (prediction), each prediction is made through stochastic feed forward pass, the meaning of which is for each sample, we randomly draw weights from posterior distribution \( T \) times, \( \hat{p}_i \) here is average probability of \( T \) feed forward pass, corresponding equation is shown in equation (2).

### 3.2.2 Expected Calibration Error (ECE)

Expected calibration error is a summarized version of reliability diagram. Basically, it uses a single scalar value to indicates the calibration error. This method also separate the predicted confidence into \( M \) groups, then it calculates the weighted average difference between accuracy and confidence in each bin, the equation is as follows [15]:

\[
ECE = \sum_{m=1}^{M} \frac{N_m}{N} |\text{acc}(I_m) - \text{conf}(I_m)|
\]

(8)

Where \( N \) is the total number of samples.

### 3.3 Ability to Tell Right or Wrong

The previous parts have mentioned the major benefit of Bayesian deep neural network is the ability to predict uncertainty. Although we expect the model could give lower average uncertainty for samples following the same distribution than the samples from a different distribution in order to help the model make a prediction with corresponding confidence boundaries. It is more rational to think about using uncertainty to provide a guidance on a prediction that should be considered as a correct prediction or a wrong prediction even it has a very high confidence score. This involves uncertainty distinguishability.

There is no doubt that we expect a sample should be given a correct prediction when the confidence score is high. However, no model can be perfect, it may give wrong prediction with very high confidence for samples from same or different distribution. Areas like medicine might have very low tolerance for such problem, a doctor would prefer the model does not give a prediction than giving a wrong prediction with high confidence. In this case, we want the uncertainty to be distinguishable under different conditions to assist making decisions. We propose two methods to estimate the distinguishability between samples from the same and from a different distribution. Additional, they could also estimate the distinguishability between correctly predicted samples and wrongly predicted samples and both samples should follow the same distribution.

### 3.3.1 Uncertainty and Probability Diagrams (UPDS)

The UPDS are visual tools to estimate the uncertainty divergence under defined conditions. These diagrams plot expected uncertainties as a function of confidence. In order to estimate the function with finite samples, we also separate samples with different prediction confidence into \( M \) groups like reliability diagrams. The average uncertainty (AU) within each interval \( I_m = \left( \frac{m-1}{M}, \frac{m}{M} \right) \) as follows:

\[
\text{AU}(I_m) = \frac{1}{N_m} \sum_{i \in N_m} \hat{u}_i
\]

(9)

Where \( N_m \) is number of samples in group \( m \), \( \hat{u}_i \) is the uncertainty (epistemic uncertainty, aleatoric uncertainty, predictive uncertainty) for sample \( i \), which is calculated by equation (3)(4). If the UPDS under two different conditions have very large divergence, especially for samples with very high confidence, it means the model is very likely to be able to provide reliable results.
3.3.2 Average Uncertainty Divergence (AUD)

Since the UPDS provide a visual way to analyze the distinguishability, it is convenient to give a scalar value to summarize it as well. Average uncertainty divergence directly calculates average difference between each group pair, and larger value indicates better distinguishability. The equation is as below:

$$AUD = \frac{1}{N_g} \sum_{i \in N_g} |\hat{AU}_a^i - \hat{AU}_b^i|$$  \hspace{1cm} (10)

Where $\hat{AU}_a^i$ means average uncertainty in group i under condition a, $\hat{AU}_b^i$ is average uncertainty in group i under condition b, $N_g$ is number of groups that have values under both conditions (some group might have None should not be considered). the AUD represents the divergence of uncertainty between different condition, which indicates the model distinguishability.

3.3.3 Scale

For classification tasks, the prediction result is the one with maximum confidence, which means the minimum confidence of this choice highly depends on the number of class in this task, for example, 10-classes problem with minimum confidence 0.1 and 2-classes problem with minimum confidence 0.5. Therefore, when we calculate the rejection ability, average uncertainty divergence and plot UPDS, especially for binary classification, the diagrams are heavily concentrated on the right side (high confidence area). Although we still can get comparable results, it is always a good idea to consider re-scale the confidence to 0 and 1. Min-Max scale is one option.

$$p_i = \frac{\hat{p}_i \cdot \frac{1}{\text{num}_\text{class}}}{1 - \frac{1}{\text{num}_\text{class}}}$$  \hspace{1cm} (11)

Where $p_i$ is scaled probability, $\hat{p}_i$ is un-scaled probability and $\text{num}_\text{class}$ is number of classes in the classification task.

4 Experimental Results

In this section, we use MNIST and Fashion-MNIST datasets tested on a 2-layer simple feed-forward neural network and LeNet to demonstrate the merit of the proposed methods. Instead of comparing the PRC, ROC and accuracy, we estimate the performance of both model through proposed perspectives.

4.1 Model Description and Datasets

As mentioned above, we trained models on MNIST training dataset, tested models on the MNIST test dataset and Fashion-MNIST test dataset. The Structures of both models are showing as follows:

![Figure 1: Network Structure](image-url)
4.2 Rejection Ability

The left diagram indicates the model performance on rejecting samples from a different distribution, and the larger the area under the curve, the more samples have low confidence score, which means more out of distribution samples can be easily rejected with a low threshold. On the contrary, the right diagram represents the model performance on accepting samples from the same distribution, the smaller the area under the curve, the more samples are predicted with a high confidence score, which means more samples with the same distribution can be accepted. The Rejection ability is calculated as equation (5).

| Model   | AUPC(DD) | AUPC(DS) | RA   |
|---------|----------|----------|------|
| Simple Net | 0.507    | 0.07     | 0.437|
| LeNet   | **0.537** | **0.023**| **0.514**|

Table 1: Rejection Ability (RA) for Simple Net and LeNet

4.2.1 Calibration Error

The reliability diagrams and ECE for Simple Net and LeNet are shown as above. For reliability diagrams, we separate samples into 10 bins, each bin has range 0.1. The number of bins for calculating the expected calibration error is set to 15. The ECE indicates that Lenet has better calibration error. Therefore, it means the probability given by LeNet is closer to the true probability than the probability given by Simple Net.

| Model   | ECE   |
|---------|-------|
| Simple Net | 0.0288 |
| LeNet    | **0.012** |

Table 2: Expected Calibration Error for Simple Net and LeNet

The reliability diagrams and ECE for Simple Net and LeNet are shown as above. For reliability diagrams, we separate samples into 10 bins, each bin has range 0.1. The number of bins for calculating the expected calibration error is set to 15. The ECE indicates that Lenet has better calibration error. Therefore, it means the probability given by LeNet is closer to the true probability than the probability given by Simple Net. Recent
researches from [5] [15] proposed ways like temperature scaling and maximum mean calibration error(MMCE) for model calibration, which could be useful for real applications. However, calibration is not the purpose of this paper, both of our models are not calibrated by these methods.

4.2.2 Ability to Tell Right or Wrong

Distinguish Samples from Different Distribution

![Uncertainty and Probability Diagrams (Different Distribution)](image)

Normally, we want to use the uncertainty to help a person or a system to make decisions. In order to do this, we want a model to be able to distinguish those samples from different distributions even they have relatively high prediction confidence. The only way to do this is to ensure the uncertainty of samples from different distributions is distinguishable to samples from the same distribution. The uncertainty and probability diagrams in Figure 4 represent such ability in a model. The diagrams show that Simple Net does not have dramatic difference on both epistemic uncertainty and aleatoric uncertainty for samples from MNIST and Fashion-MNIST, which indicates Simple net has bad distinguishability. However, for Lenet, both epistemic uncertainty and aleatoric uncertainty are quite distinguishable for samples from MNIST and Fashion-MNIST. When we take rejection ability into consideration, for example, set rejection threshold to be 0.9, almost 95 percent samples from Fashion-MNIST should be rejected and almost 95 percent samples from MNIST should be accepted. Additionally, the uncertainties for samples with confidence higher than 0.9 have clear difference, in this case, the uncertainty could be used to assist the prediction. The corresponding average uncertainty divergence (AUD) is calculated as below, and larger value indicates bigger divergence:

| Model                                           | Simple Net | LeNet  |
|-------------------------------------------------|------------|--------|
| AUD between MNIST and Fashion-MNIST (aleatoric) | 0.0019     | 0.0408 |
| AUD between MNIST and Fashion-MNIST (epistemic) | 0.0054     | 0.0370 |
| AUD between MNIST and Fashion-MNIST (predictive)| 0.0047     | 0.0097 |

Table 3: Average Uncertainty Divergence

Distinguish Samples from Same Distribution

Since no model can be perfect, and model may give wrong predictions even samples are from the same distri-
bution. In this case, uncertainty should be able to distinguish wrong predictions from the correct predictions. In this case, we intend to plot the UPDS on correctly predicted samples and wrongly predicted samples. The diagrams are shown in Figure 5. Obviously, the divergence under this condition is relatively small comparing the divergence between samples from different distributions. But still we can easily notice the aleatoric and predictive uncertainty under this condition have clear difference in LeNet for samples with confidence higher than 0.9. Therefore, LeNet model is still able to give rational predictions about whether a prediction should be trusted. The AUDs are calculated as follows:

| Model                                      | Simple Ne | LeNet |
|--------------------------------------------|-----------|-------|
| AUD between Correct and Wrong in MNIST (aleatoric) | 0.0021    | 0.0128|
| AUD between Correct and Wrong in MNIST (epistemic) | 0.0049    | 0.0059|
| AUD between Correct and Wrong in MNIST (predictive) | 0.0067    | 0.0156|

Table 4: Average Uncertainty Divergence

![Figure 5: Uncertainty and Probability Diagrams (Same Distribution)](image)

5 Conclusion

The proposed methods assess the model performance from rejection ability, calibration error and uncertainty divergence under different conditions. They provide concrete guidance to describe if a model is able to reject samples from different distribution and accept samples from the same distribution. Additionally, they also indicate if a prediction is reliable. Following these criteria, LeNet has better rejection ability, better uncertainty divergence and better calibration error than Simple Net. Last but not least, the potential reason that LeNet beats the Simple Net is that Simple Net is too simple to correctly approximate the true posterior distribution, which means the variational distribution badly underestimates the posterior comparing to the LeNet. In this case, it has worse ability to capture uncertainties from different distributions. In a word, these metrics can be very useful for comparing model performance and providing guidance to make choice for threshold along with accuracy, ROC and PRC.
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