Evaluation of Neural Network Uncertainty Estimation with Application to Resource-Constrained Platforms

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Abstract

The ability to accurately estimate uncertainties in neural network predictions is of great importance in many critical tasks. In this paper, we first analyze the intrinsic relation between two main use cases of uncertainty estimation, i.e., selective prediction and confidence calibration. We then reveal the potential issues with the existing quality metrics for uncertainty estimation, and propose new metrics to mitigate them. Finally, we apply these new metrics to resource-constrained platforms such as autonomous driver assistance systems where the quality of uncertainty estimation is critical. By exploring the trade-off between the model size and the estimation quality, a missing piece in the literature, some interesting trends are observed.

1 Introduction

A major challenge in adopting deep neural networks (DNNs) to real-world problems is the lack of self-awareness and the tendency to fail silently [Holzinger et al., 2017]. As a critical part of decision-making systems, the awareness of prediction uncertainty enables human doctors to ask for additional investigations whenever they are in doubt for a case or human drivers to slow down when they cannot clearly recognize an object. In order to transform the autonomous system from experimental tools into trusted and collaborative partners, we need to equip DNNs with self-awareness on a par with its task competency especially in mission-critical scenarios.

Most recently, much effort has been devoted to providing an accurate quantified score representing the uncertainty of the prediction [DeVries and Taylor, 2018b; Guo et al., 2017; Malinin and Gales, 2018; DeVries and Taylor, 2018a], where wrongly predicted samples are assigned with low confidence scores and correctly predicted ones are assigned with high confidence scores\textsuperscript{1}. The uncertainty estimation can either be explicitly adopted during the training processing [Lee et al., 2017b; Dhamija et al., 2018; Kumar et al., 2018] or as a post-processing step that does not affect the underlying models [Guo et al., 2017; Chen et al., 2018]. In order to evaluate the quality of various uncertainty estimation approaches, a set of metrics have been proposed in two different use cases: selective prediction [Geifman and El-Yaniv, 2017] and confidence calibration [Guo et al., 2017].

For selective prediction, the obtained confidence scores are thresholded and the model can abstain from making predictions on samples with lower confidence score to achieve higher accuracy on the remaining part [Hendrycks and Gimpel, 2016]. For instance, it is safe to defer the diagnosis of non-urgent cases to human doctors and it is more important to guarantee the accuracy of the predictions actually made. In this case, common quality metrics to evaluate uncertainty estimation are area under Receiver Operator Characteristic (AUROC) curve and area under Precision-Recall (AUPR) curve [Malinin and Gales, 2018; Hendrycks and Gimpel, 2016; Chen et al., 2018]. For confidence calibration, the aim is to provide a confidence score that approximates the probability of a prediction with this confidence score being correct. For instance, in autonomous driving, human intervention is often not available in a timely manner and the high-level planning module will need such calibrated confidence for instant decision making. In this case, common quality metrics are Expected Calibration Error (ECE) and Maximum Calibration Error (MCE) [Guo et al., 2017; Kumar et al., 2018; Sander et al., 2018].

Despite the recent advancements, it is largely unknown how/if the two main use cases of selective prediction and confidence estimation are connected. In addition, we find that the quality metrics of uncertainty estimation used by most existing works could be problematic, potentially leading to unfair comparisons, misleading results, and/or undesired learning behaviors. For selective prediction, we show that a minimal change in the prediction accuracy can make the comparison using AUROC and AUPR meaningless or even misleading. For confidence calibration, we find that ECE and MCE cannot discover some large accuracy gaps even in high confidence area. Meanwhile, they are also vulnerable to internal compensation and inaccurate accuracy estimation in each confidence interval, which lead to poor robustness and inferior accuracy.

In this paper, we first formally analyze the difference and connection between the two use cases. We then demonstrate various issues that exist in existing quality metrics, and propose new quality metrics to alleviate them. Finally, we further apply the new metrics to resource-constrained platforms.

\textsuperscript{1}Confidence is the additive inverse of uncertainty with respect to 1, so they are used interchangeably in the literature.
where the quality of uncertainty estimation is critical, such as wearable health monitoring devices and Unmanned Aerial Vehicles (UAVs). While the accuracy-resource trade-off of DNNs has been extensively studied, the trade-off between resource and uncertainty estimation quality is still missing in the literature. Our study interestingly shows that while the estimation quality for selective prediction increases significantly with the model size, that for confidence calibration is insensitive to the model size.

The main contributions of this paper are as follows

- We formally analyze the relation between the two main use cases of uncertainty estimation: selective prediction and confidence calibration, and provide new insights on their difference and interaction.
- We identify the potential issues of commonly used quality metrics for uncertainty estimation in both use cases, and propose new metrics to mitigate them.
- We apply the proposed new metrics to the important problem of uncertainty estimation in a resource-constrained scenario, and show that the quality of uncertainty estimation does not necessarily increase with the model size.
- We show that for selective prediction the estimation quality using existing metrics decreases with the model size, while that using our metric increases and is consistent with common expectation. On the other hand, the estimation quality in confidence calibration changes little with the model size.

2 Background

Various methods exist in the literature to estimate the uncertainty of neural network predictions [Gal and Ghahramani, 2016; Hendrycks and Gimpel, 2016; Chen et al., 2018; Malinin and Gales, 2018; Mandelbaum and Weinshall, 2017; Guo et al., 2017; Heo et al., 2018; Naenie et al., 2015; Kumar et al., 2018; Sander et al., 2018; Seo et al., 2018; Lakshminarayanan et al., 2017; Geifman et al., 2018; Devries and Taylor, 2018b; Dhamija et al., 2018; Lee et al., 2017b; Liang et al., 2017; Kendall and Gal, 2017]. The quality metrics to evaluate these methods can be divided into two categories depending on the use cases.

We put our discussion in a general classification setting. Following [Kumar et al., 2018], we denote \( \mathcal{Y} = \{1, 2, K\} \) as the set of class labels, \( \mathcal{X} \) as the input space, \( N_0(y|x) \) as the probability distribution of model predictions with input \( x \) and model parameters \( \theta \). For each input sample \( x_i \), the model gets a predicted label \( \hat{y}_i = \arg\max_{y \in \mathcal{Y}} N_0(y|x_i) \) and a confidence score \( r_i \). If \( \hat{y}_i = y_i \), which means the prediction is correct, we have the correctness score \( c_i = 1 \). Otherwise, \( c_i = 0 \). Then the distribution over \( r \) and \( c \) can be denoted as \( P_{\theta,D}(r,c) \). Note that we did not make any assumption on how \( c \) is obtained or any correlation between \( c \) and \( r \). Indeed, they can be obtained by any method. A model can have poor accuracy while having perfect uncertainty estimation and vice versa. As such, the two use cases can be defined as follows.

Selective Prediction With a confidence score \( r_i \) for each input \( x_i \), the model abstains from making prediction on \( x_i \) if \( r_i \) is smaller than a given threshold. AUROC and AUPR are the primary quality metrics used for selective prediction [Malinin and Gales, 2018; Mandelbaum and Weinshall, 2017; Hendrycks and Gimpel, 2016; Chen et al., 2018].

Confidence Calibration Find a confidence score \( r \in [0, 1] \) that directly reflects the probability of the prediction being correct. ECE and MCE are the primary quality metrics used for confidence calibration [Guo et al., 2017; Naenie et al., 2015; Kumar et al., 2018; Sander et al., 2018; Seo et al., 2018]. Negative Log Likelihood (NLL) and Brier Score are used as indirect and supplementary measurements in some works [Guo et al., 2017; Seo et al., 2018]. We note Brier Score and NLL are not suitable as primary metrics for confidence calibration because they prefer better prediction rather than better calibration by design.

Practically, given a finite number of samples in \( D \sim P_{\theta,D} \), ECE and MCE are calculated by partitioning the \([0, 1]\) range to \( n \) equal bins and using all samples in each bin to compute an average accuracy and an average confidence. \( n \) is chosen as 10 or 15 in the literature [Guo et al., 2017; Heo et al., 2018; Naenie et al., 2015; Kumar et al., 2018; Sander et al., 2018; Seo et al., 2018]. The difference between the average accuracy and the average confidence is the accuracy gap. Specifically, the partition is defined as \( B_j \) = \([\frac{j-1}{n}, \frac{j}{n}]\), \( j = \{1, \ldots, n\} \) and \( D_j = \{x_i | r_i \in B_j\} \). Then ECE and MCE are computed as ECE and MCE by:

\[
ECE(P_{\theta,D}) = \frac{1}{|D|} \sum_{j=1}^{n} \sum_{x_i \in D_j} c_i - \sum_{x_i \in D_j} r_i 
\]

\[
MCE(P_{\theta,D}) = \max_{j} \frac{1}{|D_j|} \sum_{x_i \in D_j} c_i - \sum_{x_i \in D_j} r_i 
\]

In addition to the quantified metric, Reliability Diagram is used as a standard qualitative tool in the literature. It indicates how ECE and MCE are obtained by plotting the accuracy as a function of confidence where each point corresponds to a bin.

An ideal accuracy-confidence curve is also marked to show the accuracy gap.

3 Relation Between the Two Use Cases

The performance of selective prediction is solely determined by the relative ranking of \( c \) and the specific values do not matter due to the thresholding mechanism. Even though a good threshold may be unknown, existing statistical methods are available for finding a desirable threshold [Geifman and El-Yaniv, 2017]. Therefore, the uncertainty estimation for selective prediction is perfect when \( r_0 > r_b \) for any \( c_0 = 1 \), \( c_b = 0 \). For confidence calibration, the quality of the confidence score is evaluated based on the difference between the confidence score and the expected accuracy of the samples with this score. Formally, the expected calibration error can be defined as:

\[
ECE(P_{\theta,D}) = E_{P_{\theta,D}(\tau)}[|E_{P_{\theta,D}(c|\tau)}[c] - \tau|] 
\]

Then uncertainty estimation for confidence calibration is perfect when \( E_{P_{\theta,D}(\tau)}[|E_{P_{\theta,D}(c|\tau)}[c] - \tau|] = 0 \).

It is interesting to see how the different objectives of the two use cases are connected with each other: It is clear that
they are not highly correlated. A confidence estimation can be perfect for one and poor for the other. We further show that a confidence estimation is perfect in both cases if and only if it perfectly knows whether each prediction is correct or wrong.

**Theorem 1.** The uncertainty estimation \( r \) is perfect for both selective prediction and confidence calibration if and only if for all samples, \( r \in \{0,1\} \), \( E_{P_{b,D}(c=0)|x} = 0 \), and \( E_{P_{b,D}(c=1)|x} = 1 \).

**Proof.** Given \( r \in \{0,1\} \), \( E_{P_{b,D}(c=0)|x} = 0 \), and \( E_{P_{b,D}(c=1)|x} = 1 \), it follows trivially that
\[
E_{P_{b,D}(c=0)|x}[E_{P_{b,D}(c=0)|x} - r] = 0 \quad \text{and} \quad r_a > r_b \quad \text{for any} \quad c_a = 1, \quad c_b = 0.
\]
On the other side, if \( E_{P_{b,D}(c=0)|x}[E_{P_{b,D}(c=0)|x} - r] = 0 \), we have \( E_{P_{b,D}(c=0)|x} = r \). If there exists \( x_i \) that \( r_i \in (0,1) \), then we have \( E_{P_{b,D}(c=0)|x} = (0,1) \). Consequently, \( \{x|c = 0, r = r_i\} > 0 \) and \( \{x|c = 1, r = r_i\} > 0 \). Then for any two samples \( x_a \in \{x|c = 1, r = r_i\} \) and \( x_b \in \{x|c = 0, r = r_i\} \), we have \( c_a = 1, c_b = 0 \) and \( r_a > r_b \) contradict the fact that \( r_a > r_b \) for \( c_a = 1, c_b = 0 \). Therefore, \( x_i \in (0,1) \). Using \( E_{P_{b,D}(c=0)|x} = r \), it follows immediately that \( E_{P_{b,D}(c=0)|x} = 0 \), and \( E_{P_{b,D}(c=1)|x} = 1 \).

4 New Quality Metrics

In this section, we discuss some potential issues of the existing quality metrics for uncertainty estimation and present new metrics to mitigate them. In all figure captions, ↑ means the higher the better. ↓ means the lower the better.

4.1 Selective Prediction

Some works get better uncertainty measured by AUROC and AUPR at the cost of slightly lower accuracy [Malinin and Gales, 2018]. However, we find that comparing AUROC and AUPR is fair only when the underlying models make the same prediction. Below we use an example to show that even a small difference in the underlying model could make the comparison of AUROC and AUPR meaningless if not misleading.

We use a 100-layer well trained DenseNet on Cifar10 as an example (Network 1). Consider a Network 2 such that the inference result of the two networks are the same except that we twist its output on the 20 most uncertain predictions among all correct ones of Network 1. As such, Network 2 gives wrong predictions with the same confidence score on these 20 samples. Note that we are only modifying 20 most uncertain samples out of 10,000 total samples, so the difference is minimal. Whenever the confidence score is used to reduce coverage, these most uncertain samples are the first to be abstained from and will not affect the performance anymore. As a result, Network 2 has a 95.1% accuracy compared with the 95.3% of Network 1. It is safe to say Network 1 is slightly better than Network 2 as it has equal or higher accuracy than Network 2 for any confidence threshold.

We plot the ROC curve and PR curve of the two networks in Figure 1 and compute the area under curve in Table 1. The curve and the area under curve for both ROC and PR consistently suggest a questionable result that Network 2 is better.

| Network 1 | AUROC↑ | AUPR↑ | AURC↓ |
|-----------|--------|--------|--------|
| 93.71     | 43.36  | 0.438  |
| 94.17     | 52.36  | 0.439  |

Table 1: Area under curve comparison. Note that Network 2 is inferior to Network 1.

The reason is that both AUROC and AUPR only measure a model’s ability to distinguish correct and wrong predictions while being blind to the model’s ability to make more correct predictions than wrong predictions. Note that the example may be extreme and the difference in many cases may not always be that significant, but when the metrics are actually used to guide training [Kumar et al., 2018], it is the gradient that matters.

To mitigate this issue, we propose to use the Risk-Coverage (RC) curve with the risk and coverage defined below in conventional notation.

\[
\text{coverage} = \frac{TN + FN}{(TN + FN + TP + FP)} \tag{4}
\]
\[
\text{risk} = \frac{FN}{(TN + FN)} \tag{5}
\]

Note that although RC curve has been used in the literature to demonstrate selective classification [Geifman and El-Yaniv, 2017], its potential use as quality evaluation of uncertainty estimation is first proposed in this work. The RC curves of Networks 1 and 2 and the associated area under RC curve (AURC) are shown in Figure 1 and Table 1. It is clear that only AURC correctly indicates that Network 2 is slightly better. The RC curve also shows that Network 2 has equal or higher accuracy on any confidence threshold.

We further show that AURC is still a good metric when the underlying model accuracy is the same because it correctly recognizes the better model just like AUROC and AUPR.

**Theorem 2.** For any two networks \( A \) and \( B \) of the same accuracy and their uncertainties measured by arbitrary methods (which can be different for \( A \) and \( B \)), the curve of \( A \) dominates that of \( B \) in the ROC space if and only if the curve of \( A \) dominates that of \( B \) in the Risk-Coverage space.

**Proof.** Proof by contradiction. Having the same accuracy means that the two networks have the same number of positive and negative samples. Suppose the curve of \( B \) dominates that of \( A \) in the ROC space but not in the Risk-Coverage space. Then there exists a point \( a \) on the curve...
of network A and a point b on the curve of B such that coverage(a) = coverage(b) and risk(a) < risk(b). From coverage(a) = coverage(b) we have $T_N a + F_N a = T_N b + F_N b$. Since $\frac{F_N a}{T_N a + F_N a} < \frac{F_N b}{T_N b + F_N b}$, we have $F_N a < F_N b$ and $T_N a > T_N b$. Remember that the numbers of positive and negative samples are equal. Therefore we have $F_P a + T_N a = F_P b + T_N b$ and $F_P a + F_N a = T_P b + F_N b$. Then we obtain $F_P a < F_P b$ and $T_P a > T_P b$. Then we have $T_P a > T_P b$ and $F_P a < F_P b$. This contradicts the fact that the curve of B is higher than that of A in the ROC space. The other direction can be proved in the same way and is omitted in the interest of space.

It is proved that a curve dominates in ROC space if and only if it dominates in PR space [Davis and Goadrich, 2006]. Therefore, the Risk-Coverage curve shares this same inherent connection with ROC curve and PR curve. When one curve does not dominate the other, AUROC, AUPR, and AURC may have different preferences. However, AURC captures the overall performance instead of only the ability to differentiate the positive samples and negative samples and is thus a more preferable primary metric.

In summary, when the underlying model accuracy is the same, AUROC is an effective quality metric to indicate the performance of selective prediction. When the model is not fixed such as being jointly trained with uncertainty objective [Mandelbaum and Weinshall, 2017; Malinin and Gales, 2018], using AUROC not only avoids potential unfair comparison but also provides another direction to maximize the performance. Another advantage of AURC is that it shows the overall performance of a selective classifier in a most human-understandable format. A non-expert can easily search for a desired operating point on the RC curve while doing that on PR curve is arguably troublesome.

### 4.2 Confidence Calibration

The accuracy and interpretability of reliability diagrams, ECE, and MCE all highly depend on the underlying binning strategy, which is overlooked by the existing literature as explained below.

**Undetectable Gap** We use the same DenseNet as an example to show the problem of the commonly used ECE, MCE, and reliability diagrams. The maximum of the softmax probability is used as the confidence score. As shown in Figure 2a, the accuracy gap on [0.9, 1] is as small as 0.0215 which means the average gap between the confidence and accuracy is 2.15%. One would expect that for confidence in this interval, the accuracy is very close to the confidence. However, as shown in Figure 2b, for input samples with confidence in [0.9, 0.91], the accuracy is only 50%. For input samples with confidence in [0.9, 0.96], the accuracy is lower than 73%. This problem can mainly be attributed to the highly non-uniform distribution of confidence and the large bin range. Most samples have a confidence score in [0.98, 1.0] and the accuracy gap on that range is small. Then an average view makes the high accuracy gap on [0.9, 0.96] undetectable by reliability diagrams, ECE, and MCE. Note that the big accuracy gap on [0.9, 0.96] by no means should be tolerated because it has higher sample density than any bins on its left and ignoring it may jeopardize mission-critical systems.

![Image](image_url)

**Figure 2:** Reliability diagram showing undetectable gap.

**Internal Compensation** Even if the confidence distribution is relatively uniform, we found that “internal compensation” can happen inside a bin and result in an overly optimistic ECE. As can be seen from Figure 2a, the gap is not always positive or negative. In fact, the different sign of the gap also exists inside a bin given a higher resolution and this makes the computed ECE lower than a more accurate one computed based on a higher resolution. Consider a toy case where half samples have $r = 0.4$, average accuracy 0.43 and the other half samples have $r = 0.5$, average accuracy 0.47. The ECE will be 0 while clearly the accurate ECE should be 0.03. We rigorously conclude this effect in Theorem 3.

**Theorem 3.** For any bin selection, $ECE(P_{\theta,D}) = ECE(P_{\theta,D})$ if and only if for any bin $B_j$, $E_{P_{\theta,D}(c|r_k)}[c] \geq r_k$ for all $r_k \in B_j$ or $E_{P_{\theta,D}(c|r_k)}[c] \leq r_k$ for all $r_k \in B_j$. Otherwise, $ECE(P_{\theta,D}) < ECE(P_{\theta,D})$.

**Proof.** For clarity, we reuse $n$, $B_j$ and $D_j$ as the number of bins, the range of bin, and the sample set where $j = \{1, \ldots, n\}$. Note that here the bin selection no longer needs to be a uniform partition. In order to make $ECE(P_{\theta,D})$ meaningful, we assume there are enough samples and $E_{P_{\theta,D}(c|r_k)}[c]$ is a solvable value. Denote the number of different values of $r$ as $m$ and these different values of $r$ as $r_k$ where $k = \{1, \ldots, m\}$. Then we partition $D$ to $m$ bins $D_k = \{x_i | r_i = r_k\}$ so that each bin only has one unique value. The ground truth ECE can be written as:

$$ECE(P_{\theta,D}) = \frac{1}{|D|} \sum_{k=1}^{m} \sum_{c \in D_k} [E_{P_{\theta,D}(c|r_k)}[c] - r_k]$$

Then we have

$$ECE(P_{\theta,D}) = \frac{1}{|D|} \sum_{j=0}^{n} \sum_{c_i \in D_j} [c_i - \sum_{x_i \in D_j} r_i]$$

$$= \frac{1}{|D|} \sum_{j=0}^{n} |D_j| [E_{P_{\theta,D}(c|r_k)}[c] - r_k]$$

Note that

$$\sum_{r_k \in B_j} |D_k|[E_{P_{\theta,D}(c|r_k)}[c] - r_k] \leq$$

$$\sum_{r_k \in B_j} |D_k|[E_{P_{\theta,D}(c|r_k)}[c] - r_k]$$

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**Image:** A diagram showing the relationship between reliability, accuracy, and ECE. The graph illustrates how changes in confidence affect accuracy and the overall performance metrics. The figure highlights the importance of understanding the distribution of confidence to avoid misleading conclusions about model performance.
and they are equal if and only if for any bin $B_j$, $E_{P_{\theta}(c|r)}[c] \geq r_k$ for all $r_k \in B_j$ or $E_{P_{\theta}(c|r)}[c] \leq r_k$ for all $r_k \in B_j$. Together with Equation 6, we conclude the proof.

**Inaccurate Accuracy Estimation** A relatively straightforward solution to the aforementioned problems is to increase the number of bins to get higher resolution on the confidence scores. However, using more bins does not always get better results. Even though $\frac{1}{|D_j|} \sum_{x_i \in D_j} c_i$ is an unbiased and consistent estimator of $E_{P_{\theta}(c|r)}[c]$ for $x_i \in D_j$, with more bins $|D_j|$ becomes smaller and the approximation becomes inaccurate and eventually this makes ECE an $L_1$ loss of the confidence score. $L_1$ loss is not suitable for evaluating confidence calibration for the same reason with Brier Score and NLL as mentioned earlier. In other words, a certain amount of internal compensation is necessary to make ECE and MCE meaningful. In fact, another loophole of the reliability diagrams and MCE is that, $\frac{1}{|D_j|} \sum_{x_i \in D_j} c_i$ may not provide accurate estimation for $E_{P_{\theta}(c|r)}[c]$ when $|D_j|$ is small. For instance, consider there is a well-calibrated model such that the gap on [0.2,0.9] are around 10%. Meanwhile, there are only 2 out of 10000 validation samples in $B_2 = [0.1,0.2]$ and one of them is correctly predicted, both reliability diagrams and MCE will show a more than 30% gap, even though the actual gap on [0.1,0.2] may be 10% given enough samples. A real example is shown in Figure 3a. In order to make the low accuracy around 0.95 visible, the number of bins is increased from 10 to 50 compared with Figure 2a. The significant fluctuation is a result of the inaccurate accuracy when the number of samples in the bin is small.

We remark that reliability diagrams suffer from the same problems as ECE and MCE discussed above due to the defective binning method. A seemingly straightforward remedy is to use equal-size binning, where each bin has the same number of samples, instead of equal-range binning. However, when the bin lies in a confidence region where samples are sparse, the resulting confidence range may be too large and less informative. On the other hand, when it lies in a region where samples are dense, the accuracy estimation may become inaccurate. This can be seen from Figure 3b and Figure 3c, when 50 and 100 bins are used respectively. From the figures, one can clearly see that a very wide bin exists in the low confidence region, and large accuracy range for those bins towards high confidence region.

To tackle this challenge, we resort to an adaptive binning strategy, where the number of samples in a bin is adaptive to the distribution of the samples in the confidence range, so that the highest confidence resolution can be used while enabling a reasonably accurate estimation of $E_{P_{\theta}(c|r)}[c]$. We denote the resulting new adaptive metrics as AECE and AMCE in the rest of this paper. We use $n = 0.25 \left( \frac{Z_{\alpha/2}}{\epsilon} \right)^2$ to estimate the number of samples needed to estimate the accuracy where $\epsilon$ is the error margin and $1 - \alpha$ is the confidence interval. We use a 80% confidence interval and let $\epsilon$ equal to the width of the confidence range of the bin in all experiments. Even though there are still two hyper-parameters, we find that the result is not sensitive to these parameters in a wide range due to its high robustness. In contrast, both equal-range binning and equal-size binning are more sensitive to the number of bins. To make it easier for other researchers to use this adaptive binning, we provide the details and our implementation as an open source tool at: https://github.com/yding5/AdaptiveBinning. It is important to note that the additional computation and memory cost is minimal and the complexity is still $O(|D|)$, so there is no scalability issue. The result is shown in Figure 3d, which achieves the best results in terms of capturing the calibration error and avoiding all the aforementioned problems. We hope researchers can use this new quality metric in confidence calibration in the future.

![Reliability Diagrams](image)

**Figure 3:** Reliability Diagrams of various binning methods.

### 5 Application to Resource Constrained Platforms

Considering that in many resource-constrained platforms such as autonomous driver assistance systems the quality of uncertainty estimation is critical, we evaluate the effect of resource constraints on the quality of neural network uncertainty estimation. Following state-of-the-art, we use maximum softmax probability [Hendrycks and Gimpel, 2016] and Temperature Scaling [Guo et al., 2017] for selective prediction and confidence calibration, respectively. Temperature Scaling uses a single positive scalar parameter $t$ called “temperature” to scale the neural network output before softmax. $t$ is selected on a randomly selected validation set by grid search.

We use two popular network structures DenseNet [Huang et al., 2017] and WideResNet [Zagoruyko and Komodakis, 2016]. For DenseNet, we keep the growth rate at 12 and reduce its depth from 100 to 10. For WideResNet, we change the widen factor of a 16-layer network and a 28-layer network.
to make it has a comparable number of parameters. Considering the practical capacity of resource-constrained platforms, we do not test networks of too large size. We evaluate the model on Cifar10 and Cifar100 to cover different levels of difficulty and accuracy. For a fixed model size, different measurements are applied to the same model. All results shown are the average of three repetitive experiments.

For selective prediction, we first show how the conventional AUPR metric changes with the model size, and the results are shown in Figure 4a and Figure 4b. It is shown that AUPR decreases with the model size, indicating networks’ decreasing capability to differentiate wrongly predicted samples and correctly prediction samples. The reason is that wrong predictions with high confidence scores, an issue known as over-confidence in high capacity neural networks [Lee et al., 2017a], are usually caused by inherent learning limitation or data similarity instead of network capacity. As a result, although higher capacity models have fewer wrong predictions, they are increasingly concentrated in the high confidence area, which in turn makes accurate uncertainty estimation harder. However, this is against the common knowledge that larger networks behave better in uncertainty estimation, the main reason being that the impact on the final accuracy in selective prediction is not taken into consideration as the network gets bigger, as discussed in Section 4.1. If we use the proposed AURC instead as shown in Figure 4c and Figure 4d, the estimation quality increases with the model size, consistent with common expectation.

For confidence calibration, the uncertainty estimation quality measured by AECE and AMCE is shown in Figure 5. We also plot the results measured by ECE and MCE in the same figures to validate the discussion in Section 4.2. We find that the estimation quality remains almost flat and does not show a strong trend with the size in terms of AECE, AMCE, ECE, and MCE. This is a mixed result of a number of factors including model accuracy, the effectiveness of Temperature Scaling and the confidence distribution.

In terms of the effect of adaptive binning, it is observed that ECE is generally smaller than AECE by a very smaller margin. The reason is that different binning methods lead to different levels of internal compensation as discussed in Section 4.2. The adaptive binning used by AECE creates an average of 12.6 and 21.2 bins for Cifar10 and Cifar100 respectively, more than the 10 equal-range bins used in ECE following the common practice in the literature. Note that Cifar100 gets more bins than Cifar10 because Cifar100 is more difficult and the confidence distribution is significantly flatter, which naturally enables more bins with accurate accuracy estimation. This further validates the superiority of the adaptive binning. Meanwhile, as shown in Figure 5c, MCE is close to AMCE for WideResnet but significantly bigger than AMCE in some cases for DenseNet. The reason is DenseNet tend to have a confidence distributions that are more concentrated to the high confidence area. As a result, the inaccurate accuracy estimation in the bins with a small number of samples is exposed and lead to some undesired big accuracy gap. This is further validated in the results on Cifar10 where both WideResnet and DenseNet have more non-uniform confidence distributions because of an easier task. As shown in Figure 5d, the MCE for both WideResnet and DenseNet are unstable and significantly higher than AMCE indicating an even worse problem caused by the inaccurate accuracy estimation.

6 Conclusions
Understanding the quality of uncertainty estimation is critical in applying neural networks to many real-world problems. In this paper, we analyzed the relation between two main use
cases of uncertainty estimation, i.e., selective prediction and confidence calibration. We further identified the issues with the existing quality metrics for uncertainty estimation, and proposed new theoretically justified metrics to mitigate them. Finally, we applied these new metrics to resource-constrained platforms and explored the trade-off between the amount of resource and the estimation quality, and made a few interesting observations.

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