EMPIRICAL CONFIDENCE ESTIMATES FOR CLASSIFICATION BY DEEP NEURAL NETWORKS

CHRIS FINLAY¹ AND ADAM M. OBERMAN¹²

Abstract. How well can we estimate the probability that the classification, \( C(f(x)) \), predicted by a deep neural network is correct (or in the Top 5)? We consider the case of a classification neural network trained with the KL divergence which is assumed to generalize, as measured empirically by the test error and test loss. We present conditional probabilities for predictions based on the histogram of uncertainty metrics, which have a significant Bayes ratio. Previous work in this area includes Bayesian neural networks. Our metric is twice as predictive, based on the expected Bayes ratio, on ImageNet compared to our best tuned implementation of Bayesian dropout [GG16]. Our method uses just the softmax values and a stored histogram so it is essentially free to compute, compared to many times inference cost for Bayesian dropout.

1. Introduction

Deep convolutional neural networks are effective at image classification tasks [SVI⁺16], achieving higher accuracy than conventional machine learning methods, but lacking the performance guarantees associated with these methods. Without additional performance guarantees, for example error bounds, they cannot be safely used in applications where errors can be costly [Pot17].

In particular, suppose a model \( f(x) \), generalizes well, so that it has a high probability, \( p \), of a correct prediction on an image \( x \) sampled from the same underlying distribution, \( \rho(x) \). In this paper we address the question of whether we can find an estimate of \( \text{Prob}(C(f(x)) = y(x)) \) the probability that the classification, \( C(f(x)) \), is the correct label, \( y(x) \).

Previous work in this area includes Bayesian neural networks. We show below that our metric is twice as predictive, based on the expected Bayes ratio, on ImageNet compared to our best tuned implementation of Bayesian dropout [GG16]. Our method also has the advantage that it is essentially free to compute (since it just uses the softmax values and a stored histogram), compared to many (30) times inference cost for Bayesian dropout.

Here \( f(x) \) is a probability vector: \( \sum_{i=1}^{m} f_i = 1 \) with each component \( f_i \geq 0 \). We write

\[
I_1(f) = \text{argmax}_i f_i, \quad M_1(f) = \text{argmax}_{f_i, f_j},
\]

for the index, and value, of the maximum component of \( f \), respectively. (In the case of a tie, choose the smallest index). The labels are represented by \( m \) one-hot label vectors \( e_k = (0, \ldots, 1, \ldots, 0) \). The classification of the vector \( f \) is given by the largest component, so write

\[
C(f) = e_m, \quad m = I_1(f)
\]

The model, \( f(x) \), is trained using the Kullback-Leibler divergence for the loss function, which corresponds to

\[
\mathcal{L}_{KL}(f, e_k) = -\log(f_k)
\]
on label vectors. Since the model is trained to minimize a loss, the values \( f_i(x) \) do not correspond to the probability that \( C(f(x)) = e_i \). However, there is a misconception that these values are not informative about the probabilities. However, values of \( f(x) \) which have a smaller loss are more likely classify correctly.

¹ Department of mathematics and statistics, McGill University
² AIFaster Consulting Inc
E-mail address: christopher.finlay@gmail.com, adam.oberman@mcgill.ca.
Date: March 25, 2019.
AO supported by AFOSR grant FA9550-18-1-0167.
The quantities of interest are the random variables $X_1$ and $X_5$ which determine if the prediction $f(x)$ is correct, or in the top 5, respectively.

Consistent with (1), use the following notation for the indices of the top 5 components in the vector $f$

$$I_5(f) = \{\text{indices of the 5 largest components of } f\}$$

again choosing the smallest indices in the case of a tie. Write $k(x)$ for the index of the correct label $y(x)$. Using this notation, define the random variables

$$X_1 = \begin{cases} 1 & \text{if } C(f(x)) = y(x) \\ 0 & \text{otherwise} \end{cases} \quad X_5 = \begin{cases} 1 & \text{if } k(x) \in I_5(f(x)) \\ 0 & \text{otherwise} \end{cases}$$

These are Bernoulli random variables with expected values corresponding to the probability of Top 1 and Top 5, respectively,

$$p_1 = \mathbb{E}[X_1], \quad p_5 = \mathbb{E}[X_5]$$

In this article we will show that we can define random variables $U_1$ and $U_5$, which we call uncertainties, whose statistics allow us to better estimate the random variables of interest $X_1$ and $X_5$. (We can also define analogous uncertainties for Top $k$ for other values of $k$ besides 1 and 5). Using the histograms of the uncertainty variables will give an improved conditional probability

$$\operatorname{Prob}(X_1(x) = 1 \mid U_1(x) = t)$$

These uncertainty variables are given by

$$U_1(x) = -\log(f_{1\text{sort}}), \quad U_5(x) = -\log\left(\sum_{i=1}^{5} f_{i\text{sort}}\right)$$

where $f_{\text{sort}}$ corresponds to the indices of $f$ sorted in decreasing order.

We make use of the the Bayes factor, which provides a metric for the effectiveness of a test in validating a hypothesis. The Bayes factor was first used by Turing in research during the second world war, (see [Goo79] and see also [Jef03]). The expected Bayes factor is discussed in [KR95].

The first example of an uncertainly variable is the loss at $f(x)$. While it is unrealistic to know the loss without knowing the correct label, we can use the loss as an illustration of the use of uncertainty variables. Note that knowing the loss does not give a certain prediction of classification error, since it is possible to have $\log(p_k(x_1)) = \log(p_k(x_2))$ with one being wrong and the other correct. However, we can accurately predict the probability correct by looking at the histogram of the loss compared to the probability correct. See Figure 1 for the histogram of the loss on ImageNet [DDS*09].

2. Uncertainty estimates

First we recall Markov’s inequality.

**Lemma 2.1** (Markov’s Inequality). For a random variable $Z$ with finite expectation, let $S \subset \{Z \geq a\}$ then

$$\operatorname{Prob}(S) \leq \frac{\mathbb{E}[Z]}{a}$$

Next we establish asymptotic confidence estimates for the uncertainty measures are given in (6).

2.1. Top 1 uncertainty.

**Definition 2.2.** Define the set where the uncertainly is small but the classification is wrong.

$$S^c = \{U_1(f(x)) \leq \epsilon \text{ and } X_1(x) = 0\}$$

**Theorem 2.3** (Confidence estimate). Measure probabilities with respect to $\rho(x)$. The probability of the set where uncertainty is less than $\epsilon$ and the classification is incorrect goes to zero with $\epsilon$. In particular

$$\operatorname{Prob}(S^c) \leq \frac{\mathbb{E}[\mathcal{L}_{KL}(f(x), y(x))]}{\log(\frac{1}{\epsilon})}$$
Figure 1. Histogram of the loss on the test set for ResNet152 on ImageNet. For $\mathcal{L}_{KL} < 0.8$ the classification is always correct. For $\mathcal{L}_{KL} > 3$ classification is always incorrect. For intermediate values, the probability correct (or Top 5) is given by the color fraction of the bin.

Proof. Claim: Let $\epsilon > 0$ be small. By assumption, $-\log f_{1}^{\text{sort}} \leq \epsilon$. Thus $f_{1}^{\text{sort}} \geq \exp(-\epsilon)$. Let $e_k$ be the correct label. Then $f_k \leq f_{1}^{\text{sort}}$, so

$$f_k \leq 1 - \exp(-\epsilon)$$

and

$$-\log(f_k) \geq -\log(1 - \exp(-\epsilon)) \geq \log(1/\epsilon).$$

Thus for $x \in S^\epsilon$, $\mathcal{L}_{KL}(f(x), y(x)) \geq \log(1/\epsilon)$.

Finally, apply Markov’s inequality to the random variable $L(x) = \mathcal{L}(f(x), y(x))$ to obtain the result. □

Remark 2.4 (Neural Networks are always overconfident). Note that the uncertainly is always less than the loss,

\begin{equation}
U_1(f) \leq \mathcal{L}_{KL}(f, e_k)
\end{equation}

with equality when $C(f(x)) = y(x)$.

2.2. Top 5 uncertainty. Let $y(x) = e_k$ be the correct label for $x$ and write

\begin{equation}
S^\epsilon_5 = \{U_5(f(x)) \leq \epsilon \text{ and } k \notin I(f, 5)\}
\end{equation}

which defines the set where the Top 5 uncertainly is small but the top 5 classification is wrong, using definition [3].

If the correct label is not in the Top 5, then the probability of the correct label, $f_k$, must satisfy

$$f_k \leq f_6^{\text{sort}}$$

with

$$f_6^{\text{sort}} \leq 1 - (f_1^{\text{sort}} + \cdots + f_5^{\text{sort}})$$

Thus the loss,

$$\mathcal{L}_{KL}(f, e_k) \geq -\log(1 - (f_1^{\text{sort}} + \cdots + f_5^{\text{sort}}))$$

Then, by an argument similar to the one for Top 1 error, we see that

\begin{equation}
\text{Prob}(S^\epsilon_5) \leq \frac{\mathbb{E}[X_5]}{\log(1/\epsilon)}
\end{equation}
3. Measuring confidence using the expected Bayes Factor

In this section we define a metric for measuring the quality of an uncertainty random variable. Suppose the random variable $U(x) \in [0, \infty)$. We can use the histogram of $U(x)$ to define bins where we measure the conditional probabilities.

3.1. The Bayes Factor. Consider a Bernoulli random variable $X = B(p_X)$. The odds for $X$ are given by $O(p) = \frac{p}{1-p}$. Now consider a test, $Y = B(p_Y)$, for which

$$p_{X,Y} = \text{Prob}(X = 1 \mid Y = 1)$$

Then the odds, given the test succeeds, are $O(p_{X,Y})$. In the odds have increased, we define the Bayes Factor to be

$$BF(X \mid Y) = \frac{O(p_{X,Y})}{O(p_X)}$$

On the other hand, if the odds have decreased, then the value of the information provided by $Y$ is to bet against, so we define the Bayes factor to be

$$BF(X \mid Y) = \frac{O(p_X)}{O(p_{X,Y})}$$

Note that the Bayes factor of a test does not depend on the probability of success for the test. Generally, we define the Bayes factor as follows. Given $X = B(p_X)$ and the test $Y = B(p_y)$, the Bayes factor for $Y$ is given by

$$BF(X \mid Y) = \max \left( \frac{O(p_{X,Y})}{O(p_X)}, \frac{O(p_X)}{O(p_{X,Y})} \right)$$

In the case where the test is certain, the Bayes factor is infinite, so we cap the odds at $T$ for a large number $T$

**Definition 3.1.** Define the regularized Bayes Factor by

$$BF(X \mid Y) = \min(T, BF(X \mid Y))$$

**Example 3.2.** For example, if $p_X = .95$ then $O(p_X) = 19$. If $p_{X,Y} = .99$ then $O(p_{X,Y}) = 99$, and $BF(X \mid Y) = 5.25$. On the other hand, if $p_{X,Y} = 2/3$ then $O(p_{X,Y}) = 2$ and $BF(X \mid Y) = 9.5$

3.2. Expected Bayes factor.

**Definition 3.3** (Histogram random variables). Next, given a random variable $U(x) \in [a, b)$ and a partition of $[a, b]$ into bins

$$a = t_0 < t_1 \cdots < t_Q = b,$$

Define the (histogram) random variables $Y_i$ corresponding to each interval

$$Y_i(x) = \begin{cases} 1 & t_{i-1} \leq U(x) < t_i \\ 0 & \text{otherwise} \end{cases}$$

so that

$$\text{Prob}(t_{i-1} \leq U < t_i) = \mathbb{E}[Y_i]$$

Each Bayes factor measures the value of information that $x$ lies in each quantile. The value of the test itself is defined to be the expected value of the Bayes factors.

**Definition 3.4** (Histogram Bayes Factors). Given $X$, $U$ and the histogram random variables $Y_i$, define the conditional probabilities

$$p_{X,i} = \text{Prob}(X = 1 \mid Y_i = 1), \quad i = 1, \ldots, Q$$
Write $BF(X \mid Y_i)$ for the regularized Bayes Factor of each $Y_i$, given by (14). The predictive value for $X$ of the random variable $U$ with respect to the histogram, is given by

$$\mathbb{E} [BF(X \mid Y_i)] = \sum_{i=1}^{Q} BF(X \mid Y_i) \mathbb{E} [Y_i]$$

### 3.3. Worked example of Bayes Factors

Consider the situation where you have exchanged phone numbers with someone, and you wish to contact them. The question is whether to send a text message or phone their number. Approximately 95% of people prefer to message. Let $X$ be the probability that a person prefers to message. The expected value and odds for $X$ is given by

$$p_X = 0.95, \quad O(p_X) = 19$$

Now suppose we have additional information, which gives these statistics based on age. Suppose we wish to predict $X$. Knowing the age $U$ has a value. Let $U(x)$ be the age, and consider three bins for $U$ given by the values 20, 65 and let $Y_1, Y_2, Y_3$ be the corresponding histogram random variables.

$$\begin{cases} 
Y_1 = 1_{\{U < 20\}}, & \mathbb{E} [Y_1] = .4 \\
Y_2 = 1_{\{20 \leq U \leq 65\}}, & \mathbb{E} [Y_2] = .5 \\
Y_3 = 1_{\{65 < U\}}, & \mathbb{E} [Y_2] = .1 
\end{cases}$$

Since older people are more likely to prefer to use a phone, the conditional probabilities and corresponding odds are given by

$$\begin{cases} 
p(X \mid Y_1) = .999, & O(p_{X,Y_1}) = 999 \\
p(X \mid Y_2) = .94, & O(p_{X,Y_2}) = 15.7 \\
p(X \mid Y_3) = .9, & O(p_{X,Y_3}) = 9 
\end{cases}$$

In particular, knowing if they are younger or older is more valuable than the middle range. The Bayes ratio (relative odds) expresses the value of knowing the age if someone is willing to bet with the odds $O(p_X)$. So this information allows an expected profit on the bet given by the ratio.

$$\begin{cases} 
BF(X \mid Y_1) = 999/19 = 53 \\
BF(X \mid Y_1) = 19/15.7 = 1.2 \\
BF(X \mid Y_1) = 19/9 = 2.1 
\end{cases}$$

So the value of the information depends on the cases. Finally, if we wish to find the expected value of the information, we take an expectation with respect to the probabilities of the events.

$$\mathbb{E} [BR(X \mid Y_i)] = 53 \times .4 + 1.2 \times .5 + 2.1 \times .1 = 22$$

Some other information about the person may be much less useful in prediction their preference. For example, suppose you know the region where they live and let $Y_1, Y_2, Y_3$ be the histogram random variables. Suppose

$$\begin{cases} 
p(X \mid Y_1) = .03 & \mathbb{E} [Y_1] = .3 \\
p(X \mid Y_2) = .05 & \mathbb{E} [Y_2] = .5 \\
p(X \mid Y_3) = .07 & \mathbb{E} [Y_3] = .3 
\end{cases}$$

Since $\mathbb{E} [X] = .95$,

$$\begin{cases} 
BF(X \mid Y_1) = 1.9 \\
BF(X \mid Y_1) = 1.1 & \mathbb{E} [BF(X \mid Y_i)] = 1.5 \\
BF(X \mid Y_1) = 1.3 
\end{cases}$$

So with an expected value of 1.5, compared to age, with an expected value of 22, the location information is much less valuable.
Figure 2. Bayes ratio over equal 20 quantile bins on test set for ImageNet: loss, entropy, $U_1$, $U_5$. The entropy and $U_1$, $U_5$ have very large Bayes ratio in the first 10 and last 3 bins.

Table 1. Regularized Bayes ratio $E[BR]$ against various measures of confidence. For CIFAR-10 we used $X_1$, the probability of the correct label; for CIFAR-100 and ImageNet-1K we used $X_5$, the probability that the correct label is in the Top5. The mean is reported over 10-fold cross-validation of the test set.

| Confidence measure         | CIFAR-10 | CIFAR-100 | ImageNet-1K |
|----------------------------|----------|-----------|-------------|
| Model Entropy              | 150.03   | 120.40    | 37.53       |
| $- \log p_{\text{max}}$   | 141.56   | 131.38    | 44.97       |
| $- \log \sum p_{1:5}$     | -        | 106.69    | 52.39       |
| $\|\nabla_x \|_p$         | 264.85   | 132.37    | 45.89       |
| Dropout variance ($p = 0.002$) | 239.92   | 99.36     | 24.15       |
| Dropout variance ($p = 0.01$)   | 172.86   | 31.09     | 34.76       |
| Dropout variance ($p = 0.05$)   | 19.77    | 1.39      | 1.57        |
| Loss                       | $\infty$| 782.45    | 549.94      |

4. Empirical Results

4.1. Bayes Ratio. In Figure 4.1 we plot the regularized Bayes ratio for our two main measure of confidence, $U_1$ and $U_5$ along with the loss and the model Entropy. The entropy and $U_1$, $U_5$ have very large Bayes ratio in the first 10 and last 3 bins. In Table 2 we show the expected Bayes ratio for various confidence measures, on CIFAR-10, CIFAR-100, and ImageNet-1K. In addition to the confidence measures already discussed, we considered Bayesian dropout, and the norm of the gradient of the model.

In Figure 4.1 we plot the histogram bins of the model entropy against the Top 1 and Top 5 correct. From these bins, we can read of the probabilities, and output predictions for unknown images drawn from the same distribution.

4.2. Confidence bins. In this section we present confidence bins for ImageNet-1K. These bins are concise summaries of the information presented in the larger bins. Table 2 presents short bins for ImageNet. Bins for CIFAR-10 and CIFAR-100 are given in Tables 4 and 8 respectively.
Figure 3. Top 1 (green) and Top 5 (green or blue) probabilities conditioned on the 20 histograms bins of the entropy on test set for ResNet152 on ImageNet. The Top 1 probability conditioned on the first 12 bins is very close to 100%. The Top 5 probability is no better than 50% on the last few bins. The intermediate bins are less informative.

Table 2. Confidence bins for ImageNet-1K. The values of $a$ and $b$ are chosen such that $P(\text{top5} \mid Y < a) = 0.99$ and $P(a \leq \text{top5} \mid Y < b) = 0.95$. For the model used here, $P(\text{top5}) = 0.9406$.

| Confidence measure $Y$ | $(a, b)$ | $P(Y < a)$ | $P(a \leq Y < b)$ | $P(Y \geq b)$ |
|------------------------|----------|-------------|-------------------|---------------|
| Model Entropy          | (0.31, 1.40) | 0.55        | 0.31              | 0.14          |
| $- \log p_{max}$       | (0.047, 0.41) | 0.52        | 0.26              | 0.22          |
| $- \log (p_1 + \cdots + p_5)$ | (6.2e−3, 0.03) | 0.66        | 0.13              | 0.21          |
| $\|\nabla_x \|p\|$     | (0.19, 0.30) | 0.52        | 0.08              | 0.40          |
| Dropout variance ($p = 0.002$) | (8.5e−4, 4.7e−3) | 0.50        | 0.15              | 0.35          |

Table 3. Confidence bins for CIFAR-100. The values of $a$ and $b$ are chosen such that $P(\text{top5} \mid Y < a) = 0.99$ and $P(a \leq \text{top5} \mid Y < b) = 0.95$. For the model used here, $P(\text{top5}) = 0.916$.

| Confidence measure $Y$ | $(a, b)$ | $P(Y < a)$ | $P(a \leq Y < b)$ | $P(Y \geq b)$ |
|------------------------|----------|-------------|-------------------|---------------|
| Model Entropy          | (0.082, 2.1) | 0.24        | 0.50              | 0.26          |
| $- \log p_{max}$       | (7.9e−3, 0.42) | 0.24        | 0.49              | 0.27          |
| $- \log \sum p_{1:5}$ | (4.8e−3, 0.34) | 0.19        | 0.57              | 0.24          |
| $\|\nabla_x \|p\|$     | (0.46, 1.70) | 0.27        | 0.17              | 0.56          |
| Dropout variance ($p = 0.002$) | (6.4e−4, 2.2e−3) | 0.27        | 0.06              | 0.67          |

5. Extensions

In this section we discuss some extensions of the confidence results. We show that we can detect mislabeled images in the test set. We also show that we can obtain some confidence results for off manifold images, as well as adversarial images.
Table 4. Confidence bins for CIFAR-10. The value of \( a \) is chosen such that \( P(\text{top1} | Y < a) = 0.975 \).

| Confidence measure \( Y \)         | \( a \) | \( P(Y < a) \) | \( P(Y \geq a) \) |
|-----------------------------------|--------|----------------|-----------------|
| Model Entropy                     | 1.6    | 0.95           | 0.05            |
| \(- \log p_{\text{max}}\)        | 0.57   | 0.95           | 0.05            |
| \( \| \nabla_x \|_p \| \| \)     | 8.16   | 0.93           | 0.07            |
| Dropout variance (\( p = 0.002 \))| 0.045  | 0.92           | 0.08            |

Figure 4. Illustration of uncertainty measures on ImageNet. Left: entropy vs loss on the test set. Right: frequency plot of model entropy.

Figure 5. Confidence on ImageNet with Bayesian Dropout, Frobenius norm of model variance with dropout probability \( p = 0.002 \).
5.1. Detection of mislabeled images. We are able to detect test images which are mis-labeled: images which the network correctly classified, but who’s label is incorrect, or for which multiple labels could apply. These are images with high loss but low model entropy. For example in Figure 6 we show six images from the ImageNet-1k test set who’s predictions where not in the top5, but had low model entropy. All six of these images either have an incorrect dataset label, or could be described by multiple labels.

5.2. Confidence on out-of-distribution and adversarial images. Next we studied whether we could detect out-of-distribution images generated by COCO. In figure 7 we show how the histogram of the model entropy is shifted to the right compared to the on-distribution images. Table 5 give the results of our test: choosing a confidence measure which rejects 10% of the on-distribution images, our confidence measures rejected as much as 38% of COCO images (for Entropy) with similar values for $U_1, U_5$. On the other hand Dropout was completely ineffective.

Finally, we tested our confidence measures on adversarially perturbed images. In this case the gradient norm detected 50%.

REFERENCES

[DDS+09] Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In 2009 IEEE conference on computer vision and pattern recognition, pages 248–255. Ieee, 2009.
Table 5. Discarding out-of-distribution images from ImageNet-1K. For each confidence measure $Y$, the value of $a$ is chosen such that $P(Y \leq a \mid \text{image is from ImageNet-1k}) = 0.9$. Evasive attack penalizes both model entropy and gradient with Lagrange multiplier 0.1.

| Image source       | Confidence measure       | $a$   | $P(\text{image discarded})$ |
|--------------------|--------------------------|-------|-----------------------------|
| COCO               | Model Entropy            | 1.75  | 0.38                        |
|                    | $- \log p_{\text{max}}$ | 0.77  | 0.34                        |
|                    | $- \log \sum p_{1:5}$   | 0.13  | 0.37                        |
|                    | $\|\nabla x \| p \|\|$   | 1.06  | 0.23                        |
|                    | Dropout variance ($p = 0.002$) | 0.024 | 0.0                          |
| adversarially      | Model Entropy            | 1.75  | 0.28                        |
| perturbed ($L_2$)  | $- \log p_{\text{max}}$ | 0.77  | 0.25                        |
|                    | $- \log \sum p_{1:5}$   | 0.13  | 0.28                        |
|                    | $\|\nabla x \| p \|\|$   | 1.06  | 0.58                        |
|                    | Dropout variance ($p = 0.002$) | 0.024 | 0.39                        |

[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.

[Goo79] Irving J Good. Studies in the history of probability and statistics. XXXVII AM Turing’s statistical work in world war ii. Biometrika, pages 393–396, 1979.

[Jeff3] Harold Jeffreys. Theory of probability, 3rd Edition. Oxford Classic Texts in the Physical Sciences. Clarendon Press, 3 edition, 2003.

[KR95] Robert E Kass and Adrian E Raftery. Bayes factors. Journal of the American Statistical Association, 90(430):773–795, 1995.

[Pot17] Richard Potember. Perspectives on research in artificial intelligence and artificial general intelligence relevant to DoD. Technical report, The MITRE Corporation McLean United States, 2017.

[SVI16] Christian Szegedy, Vincent Vanhoucke, Sergey Ioffe, Jonathon Shlens, and Zbigniew Wojna. Rethinking the Inception Architecture for Computer Vision. In 2016 IEEE Conference on Computer Vision and Pattern Recognition, CVPR 2016, Las Vegas, NV, USA, June 27-30, 2016, pages 2818–2826, 2016.