Bayesian Neural Networks with Soft Evidence

Edward Yu
Genesis Global Trading
New York, NY 10003
eyu@genesistrading.com

Abstract

Bayes’s rule deals with hard evidence, that is, we can calculate the probability of event $A$ occurring given that event $B$ has occurred. Soft evidence, on the other hand, involves a degree of uncertainty about whether event $B$ has actually occurred or not. Jeffrey’s rule of conditioning provides a way to update beliefs in the case of soft evidence. We provide a framework to learn a probability distribution on the weights of a neural network trained using soft evidence by way of two simple algorithms for approximating Jeffrey conditionalization. We propose an experimental protocol for benchmarking these algorithms on empirical datasets, even when the data is purposely corrupted.

1 Introduction

In a traditional probabilistic reasoning framework, we make inferences based on hard evidence, or in other words, observation of some event $B$. Then we may be able to say something about the likelihood of another event $A$ by calculating $P(A|B)$. Take the classic case of Bernoulli trials, in which we are flipping a (possibly biased) coin multiple times. Each flip of the coin constitutes hard evidence, as we are certain whether the coin landed heads or tails, and we can record the event definitively: either $B = 1$ or $B = 0$. Then we may use a traditional Bayesian framework to estimate the probability the next flip will result in heads or tails.

In contrast, soft evidence arrives in the form of another probability distribution $R(B)$ as described by Peng et al. [17], or more simply, as an “unreliable testimony” of $B$ accompanied by a strength of belief in the $[0, 1]$ interval as in Chan and Darwiche [5] and Jacobs [12]. In the example of Bernoulli trials, imagine that in poor visibility conditions we are not able to ascertain definitively whether the coin landed heads or tails, but we estimate that there is a 80% probability it landed heads, i.e., $R(B = 1) = .8$. Soft evidence appears in many real world contexts, from unreliable witness testimonies in murder trials [9] to game theoretic decision making [8].

In such cases, there is no consensus on how to update one’s beliefs in order to calculate $P(A|B)$, or in a generalized machine learning setting, how to train models given soft evidence. One sensible approach is Jeffrey’s rule of conditioning [13] [19], which can be thought of as an modification of the posterior probability distribution given a set of constraints. For a Bernoulli constraint, Jeffrey’s rule reduces to standard probabilistic reasoning in the case where we observe $B$ with probability $R(B) = 1$, and is otherwise a convex combination of $P(A|B = 1)$ and $P(A|B = 0)$. Although it seems natural to interpret soft evidence in this way, it is of philosophical debate (beyond the scope of this paper) whether it is “correct”. Suffice it to say that there are both many extensions of Jeffrey’s original rule [11] [11] [2] [21], and alternative approaches based on the broader field of Dempster-Shafer theory [20] [17].

There are several related areas of study when it comes to applying soft evidence to practical machine learning domains. Pearl’s method is another method of dealing with soft evidence, whereby a Bayesian network is extended with an additional node, and soft evidence is recast as hard evidence of a virtual event. In fact, Chan and Darwiche [5] show that one may convert between Pearl’s method
and Jeffrey’s method by specifying likelihood ratios. Peng et al. [17] extend this work from theory to application by providing several algorithms for approximating Jeffrey’s method on Bayesian networks. We in turn build upon Peng et al. [17] and extend the algorithms for usage in neural networks.

A related field is that of learning noisy labels, where data is given in the form \( \{x_i, y_i \sim R(y)\} \), however unlike the soft evidence case where \( R(y_i) \) is given, in the noisy label case only \( y_i \) is observed. Rolnick et al. [18] posit that under certain types of noise, the noisiness of the labels can be ignored and a neural network is trained as if the noise did not exist. Karimi et al. [14] give a survey of methods for dealing with label noise, from label preprocessing to weighted loss functions. Since soft evidence can be converted to a noisy label by taking \( y_i = \text{arg max}_\gamma R(\gamma) \), we use methods from learning noisy labels as baselines.

The main contributions of this paper are:

1. To our knowledge, we are the first to extend Jeffrey conditionalization to the training of neural networks. We combine algorithms from computational statistics and standard Bayesian neural network training into a complete methodology for learning Bayesian neural networks that are capable of handling soft evidence.
2. We focus on practical applications, including two approximation methods for Jeffrey’s method: one simple ensemble method and one method based upon the IPFP algorithm.
3. We devise a methodology for fair benchmarking against state of the art methods in related domains, including baselines such as ensembles which ignore the soft evidence and training methods for noisy labels.

The rest of the paper is organized as follows: Section 2 defines Jeffrey’s rule and gives an example. Section 3 gives two approximation algorithms for learning neural networks using Jeffrey’s rule. Section 4 defines the experimental protocol, including evaluation criteria, methodology for generating corrupted data, baseline models, and preliminary results.

2 Jeffrey’s rule of conditioning

Consider an original probability distribution \( P(\alpha) \) which we wish to update when we receive soft evidence that arrives in the form of another probability distribution \( R(\gamma) \), where the set of mutually exclusive events \( \gamma_1, ..., \gamma_n \) is contained in the set \( \alpha_1, ..., \alpha_n \). Jeffrey’s rule gives a new updated distribution

\[
J(\alpha) = \sum_{i=1}^{n} R(\gamma_i) \frac{P(\alpha, \gamma_i)}{P(\gamma_i)} = P(\alpha|\gamma_i)R(\gamma_i)
\]  

(1)

Jeffrey’s rule gives the unique distribution that follows the principle of probability kinematics [5], that is, for all events \( \alpha \), it is the case that

\[
J(\alpha|\gamma_i) = P(\alpha|\gamma_i) \text{ for } i = 1, ..., n
\]  

(2)

Rephrased, Jeffrey’s rule finds the closest distribution (minimum KL-divergence [17]) to \( P \) that satisfies the constraints \( R \).

3 Jeffrey’s and neural networks

Now consider a Bayesian neural network with weights \( w \) and data \( D = \{(x_i, R(y_i))\} \). The posterior predictive distribution is

\[
p(y|x, D) = \int p(y|x, w)p(w|D)dw
\]  

(3)

Under an i.i.d assumption, define

\[
R(D) = \prod_i R(y_i)
\]  

(4)

We would like to obtain a Jeffrey neural network given by

\[
J(y|x) = \sum_k p(y|x, D_k)R(D_k)
\]  

(5)
Unfortunately this is computationally intractable as this would require enumerating through all permutations of $D_k$, and training a separate neural network for each permutation. We give the following two algorithms as practical alternatives.

### 3.1 Top K approximation

We limit ourselves to training $K$ neural networks as computational resources permit.

**Algorithm 1:** Top K approximation

```plaintext
foreach $k = 1, 2, ..., K$ do
    Draw sample $D_k \sim R(D)$;
    Train Bayesian neural network $p(y|x, D_k)$;
end

Ensemble is then $\bar{J}(y|x) = \frac{\sum p(y|x, D_k) R(D_k)}{\sum R(D)}$
```

Since $E[D_k] = E[R(D)]$, $E[\bar{J}(y|x)] = E[J(y|x)]$ and $\bar{J}(y|x)$ is an unbiased estimator. This can be seen as a generalization of bagging [4], whereas in the bagging procedure we sample uniformly from the empirical distribution $\hat{R}(D)$, and therefore all possible $D_k$ have equal probabilities of being sampled.

### 3.2 Iterative proportional fitting procedure

If only one neural network is to be trained, then we may approximate Jeffrey’s rule by the IPFP algorithm. The algorithm was first devised by Deming and Stephan [6] all the way back in 1940, and extended to Bayesian networks by Peng et al. [17]. The idea is to iteratively perturb the initial distribution $J_0(y)$ closer and closer to the constraints $R(y)$, one constraint at a time until convergence. This approach is powerful as $R(y)$ and $J(y)$ can be any two arbitrary distributions and need not come from the same family.

**Algorithm 2:** IPFP-NN

```plaintext
Let $J_0(y|x)$ be a neural network trained on $D = \{(x_i, \arg\max_y R(y_i))\}$;
Let $R(z) = \{R(z')\}$ be a set of constraints for a given $x_i$;
foreach $x_i$ do
    foreach $k = 1, 2, ...$ do
        foreach $z_j$ do
            if $J_{k-1}(z_j|x_i) > 0$ then
                $J_k(y|x_i) = J_{k-1}(y|x_i) \frac{R(z_j)}{J_{k-1}(z_j|x_i)}$
            else
                $J_k(y|x_i) = 0$
            end
        end
    end
    Append to data: $D = D \cup (x_i, \arg\max_y J_k(y_i|x_i))$;
end
Train final neural network $J_{k+1}(y|x)$ on $D$
```

### 4 Experimental protocol

The general procedure is as follows:

1. Select standard dataset $D = \{(x_i, y_i)\}$.
2. Convert to probabilistic dataset $D = \{(x_i, R(y_i))\}$ by purposefully generating noisy labels.
3. Evaluate model on accuracy and calibration metrics, attempting to keep computing resources equal for all models.
We will evaluate on three (modified) classification datasets: MNIST, SVHN, and ImageNet.

4.1 Evaluation criteria

Our goal is not to beat state-of-the-art benchmarks on the datasets, but rather to show an improvement in both/either loss or calibration metrics over the baseline models. A well calibrated model is one that is correct on high confidence predictions and incorrect on low confidence predictions. The Expected Calibration Error \[10\] \[15\] is found by segregating the model predictions into \(M\) bins sorted by the predictor’s confidence and looking at the gap between the accuracy and confidence. Define accuracy as

\[
\text{acc}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} \mathbb{1} (\hat{y}_i = y_i),
\]

where \(\hat{y}_i\) is the most likely predicted label \(\arg \max_y J(y|x_i)\) and \(y_i\) is the most likely true label \(\arg \max_y R(y)\). Define confidence as

\[
\text{conf}(B_m) = \frac{1}{|B_m|} \sum_{i \in B_m} R(\hat{y}_i)
\]

\[
ECE = \sum_{m=1}^{M} \frac{|B_m|}{|D|} \left| \text{acc}(B_m) - \text{conf}(B_m) \right|
\]

We will use ECE as our primary metric for calibration, and negative log likelihood as our primary loss function.

4.2 Generating corrupted datasets

In the classification setting with a hard evidence label \(y_i = C\), \(R(y_i)\) is a categorical distribution with \(R(y_i = C) = 1\) and 0 otherwise. We set a corruption index \(H\), generate a new categorical distribution \(\tilde{R}(y_i)\) with uniform random noise in the range \([-H, H]\) added to \(R(y_i)\), and renormalize as necessary. We will run experiments with \(H = .1, H = .5,\) and \(H = .9\).

4.3 Models and baselines

For all methods, we set a common base learner: a neural network with a fixed architecture trained via the Bayes by Backprop algorithm \[3\]. Since some of the methods are ensembles and others train on a larger, generated dataset, we will attempt to offer a fair comparison by using the same number of compute hours to perform hyperparameter search and train each model. We will compare the following methods:

1. Top K approximation to Jeffrey’s (TOPK): see algorithm [1]
2. IPFP-NN method (IPFP-NN): see algorithm [2]
3. Noisy labels (NL): train on \(D = \{(x_i, \arg \max_y R(y_i))\}\).
4. Noisy labels ensemble (NLE): train on \(D = \{(x_i, \arg \max_y R(y_i))\}\) using K base learners, and output the majority vote class.
5. Bagging (BAG): For each \(x_i\), draw multiple \(y^l_i \sim R(y_i)\), train using augmented dataset of size \(L \times |D|\).
6. Confident learning (CL): Discard all training data where \(\arg \max_y R(y_i)\) is less than some threshold, train using the reduced dataset. This simplistic approach is possible because of the soft evidence that is available. See Northcutt et al. [16] for confident learning in the case where \(R(y)\) must be estimated.

4.4 Preliminary evaluation

As a sanity check, we implement both algorithms using a simple statistical model in a Bernoulli trial problem setting. Assume we have a biased coin and we want to estimate its parameter \(\theta\), with the true parameter having value \(\theta = .7\). We flip the coin 1000 times and record each trial \(y_i\). However, we
do not observe $y_i$ directly but rather observe a noisy observation $R(y_i)$ by adding uniform random noise as described in section 4.2, with corruption $H = .5$. We implement algorithms 1 and 2 and plot the posterior $p(\theta | D)$ below. Note that we should not expect the MAP estimate to be at $\theta = .7$, as we have flipped the most likely label in some trials by corrupting $R(y_i)$. We use a Beta(1, 1) prior and assume a beta likelihood as well.

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