Bayesian Neural Networks

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Abstract

Bayesian Neural Networks are...

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2 Machine Learning

Machine learning includes a variety of topics of which artifical intelligence (AI) and neural networks are a subset. Neural networks in particular involve an abstract imitation of the human brain using simulated neurons which is trained on data using particular algorithms.

The term supervised learning refers to a specific common method of machine learning that uses a labeled dataset to train a model to correctly predict the labels via some training algorithm. A classification problem in supervised learning involves predictions where all labels are grouped into a set of categories. The training process can be broken down into three major steps, which include a decision process, an error function, and an optimization process [7]. The decision process is the set of steps the algorithm takes after receiving the data based on the goal of the model. The second step in the process is the error function, which is the method of measuring chosen to see if the algorithm gave a “good" or “bad" input. The two most common choices of the error function are a simple yes or no on whether a data point was classified correctly in the case of classification, or the difference in value between the predicted outcome and the actual observed outcome for continuous values. Finally, the third and last step is the part of the process that implements learning. This step, the updating or optimization process, requires the algorithm to review the past data and outputs of the error function in order to better correct its decision-making process in the future.

Throughout this report, we will often use the terms machine learning, deep learning, and neural networks. It is important to note that although these are fundamentally related fields, deep learning is a subfield of neural networks that in particular focuses on more complicated neural networks, while neural networks are a subfield in machine learning.

We will be training a classifier on labeled images in a supervised learning process to predict what is depicted in the image from a range of possibilities such as dog, cat, and plane. These images come from the CIFAR-10 dataset, which will be discussed more in detail later in this paper.

2.1 Neural Network

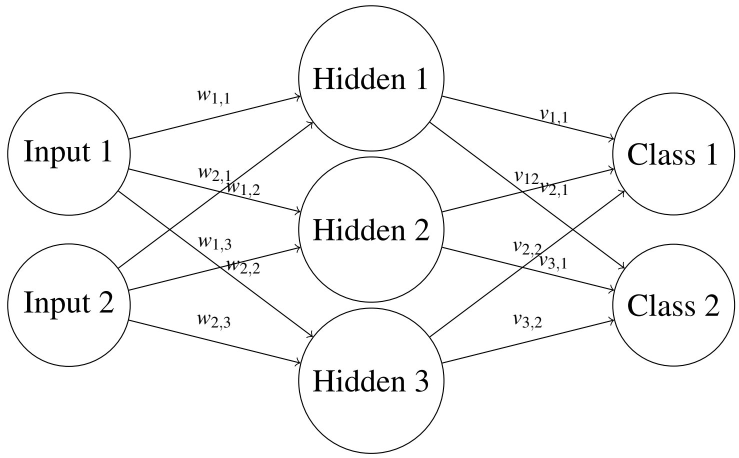


Figure 1: Example neural network

A neural network takes a series of inputs. An example of a neural network with two inputs, one hidden layer of size three, and two outputs appears in figure 1

2.2 Neural Network Neurons

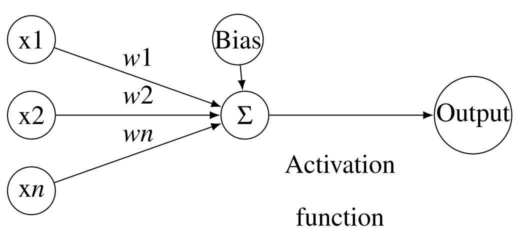


Figure 2: Neural network neuron

Neural networks are made out of a series of neurons... The neurons take a set of inputs, multiplies the inputs by the weights, sums the weighted input, adds a bias, and runs the output through an activation function...

2.3 Convolutional Neural Networks

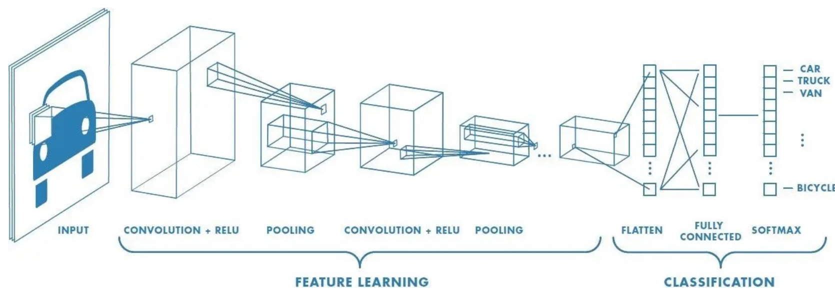


Figure 3: CNN pipeline [4]

Convolutional neural networks (CNN) are a type of neural network that is better suited for image recognition. While this might sound like a seperate model structure, CNNs are largely the same. In figure 3 the difference between a traditional neural network is the convolutional layer. Instead of reading the entire image at once, a convolutional layer slides over the image...

IMAGE OF SLIDING (gif split)

3 Bayesian Neural Networks

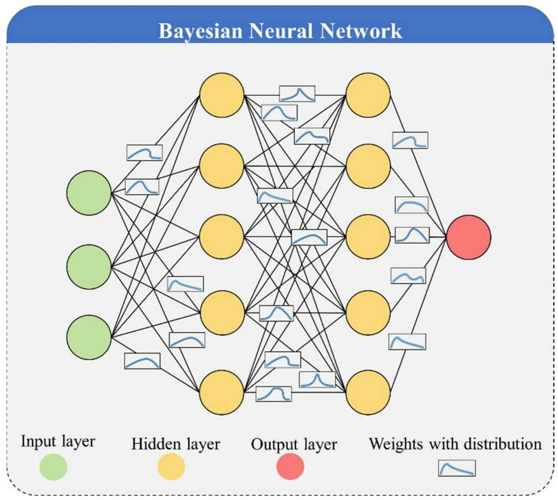


Figure 4: Example BNN [1]

Bayesian neural networks (BNN) take the same principle as your typical neural network, but factor in a measure of uncertainty into the prediction of the network. This uncertainty, of course, comes from the Bayesian theory of statistics, which believes that all events have some level of randomness, and thus must have uncertainty in their prediction.

One way this uncertainty can be built into the model is through a prior probability distribution. Uncertainty estimates of the model can be obtained from the parameters of the BNN in their probability distributions [6]. The average estimate of the parameters is computed through multiple different models during the training process, which can regularize the network. However, it can be very difficult to calculate the model posterior of a BNN. Approximations of the posterior of the model are most often used, but those are often still very computationally intensive. Different methods of approximating the model's posterior is a current research topic within the field.

The two main types of uncertainty within a BNN are aleatoric uncertainty and epistemic uncertainty. Aleatoric uncertainty is a measure of the uncertainty in the observations, which is uncertainty that is inherent in any form of data. This type of uncertainty is modeled by placing a prior distribution over the output of the BNN model. In contrast, epistemic uncertainty is a measure of the uncertainty caused by the model and its predictions. It is modeled by a prior distribution over the model's weights, and an analysis of how much the weights of the model change when the data given to the model changes [6].

But what is so great about calculating uncertainty in our model? Well, it's that our predictions become more uncertain. One of the major issues with neural networks as they are is they are highly prone to overfitting the data. Although they are great at predictions on the training data they are given, they often struggle with predictions on the testing data they are given due to the issue of overfitting. Many methods have been developed in order to regularize neural networks to work to prevent this from occurring, such as weight control measures. Using the Bayesian framework of uncertainty and building it into a model serves as a built-in prevention of overfitting.

3.1 Bayesian Neural Network Neuron

Similar to a neural network such as...

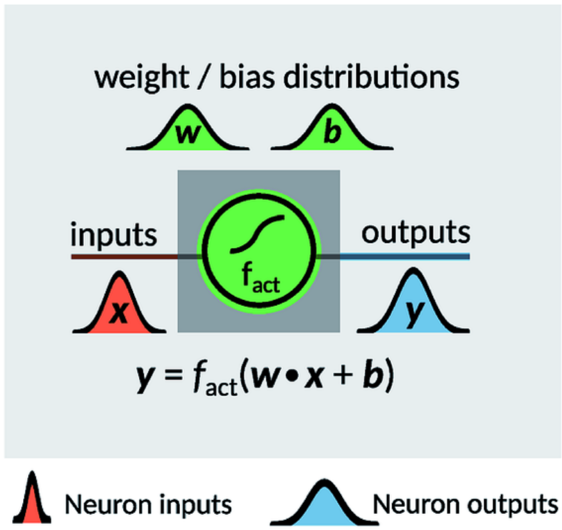


Figure 5: Example BNN Neuron [2]

3.1.1 Priors

This section was requested by Micheal.

3.2 Bayesian Convolutional Neural Networks

Bayesian convolutional neural network (BCNN) are similar to CNNs. The difference between is that BCNNs and a CNN is that the BCNN uses a bayesian neuron.

4 Simulation

We use a BCNN implementation from Github based on work from ... [6] [5]

4.1 CIFAR-10

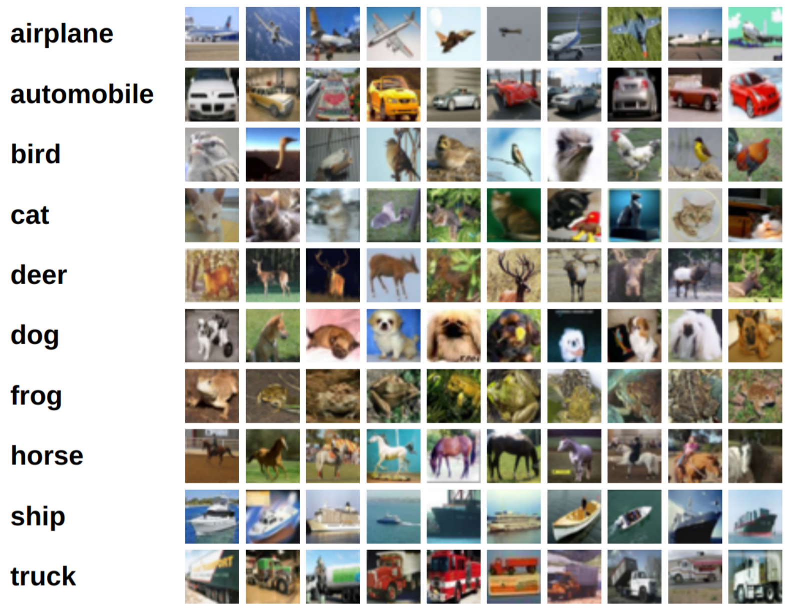


Figure 6: Example CIFAR-10 images [3]

The CIFAR-10 (Canadian Institute For Advanced Research 10) dataset is a machine learning benchmarking set. It contains $60,000$ 32×32 RGB pictures of airplanes, cars, birds, cats, deer, dogs, frogs, horses, ships, and trucks [3]. The ten classes within the dataset are mutually exclusive, meaning there is no image containing multiple of the objects mentioned above. The number of images is split evenly between each class, with $6,000$ images per each type of object. It is a very popular data set (in fact the most common) to use in machine learning and training neural networks, due to the extensive size, as well as the decent number of categories. The purpose of the images within the dataset being of a lower resolution is to allow researchers to see more quickly (and with less computation effort) how well an algorithm works on classification with the dataset. Convolutional neural networks are often seen to be the “best" at classifying CIFAR-10.

4.2 Hyperparamaters

We used the following hyperparamaters for training:

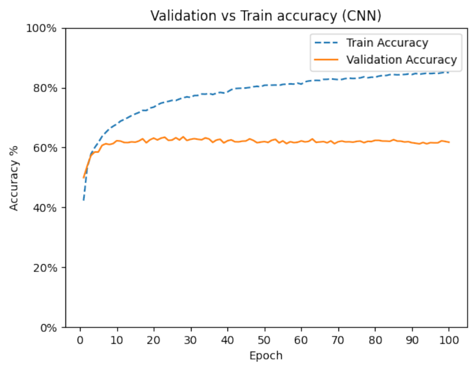
Hyperparameter	**CNN**	**BCNN**
Epochs	100	100
Learning Rate	0.001	0.003
Regularization Rate	0.001	0.001
Optimizer	Adamw	Adamw

In addition to the hyperparamaters above, the two models have the same number of layers and levels. We did not adjust the priors, as those were set by the BCNN layer code from [5].

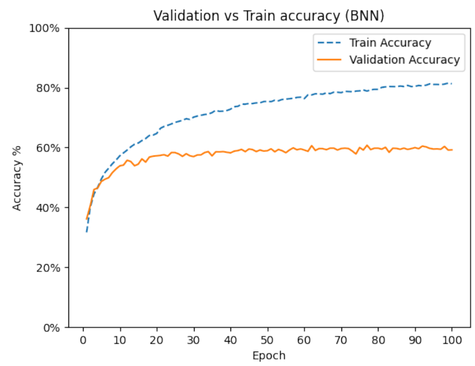
4.3 Results

Metric	**CNN**	**BCNN**
Train Accuracy	84.96%	81.27%
Validation Accuracy	61.76%	59.21%
Time to Train	16 min 11 sec	22 min 11 sec

The results we achieved with training were about the same between the BCNN and the CNN. However, the bayesian model took longer to train.



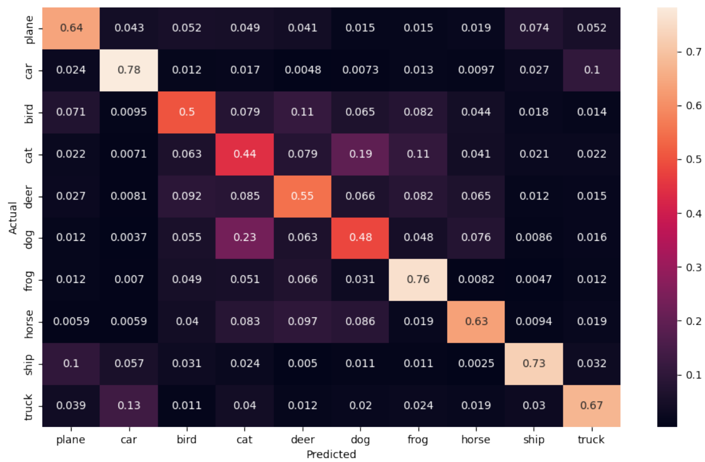
(a) CNN



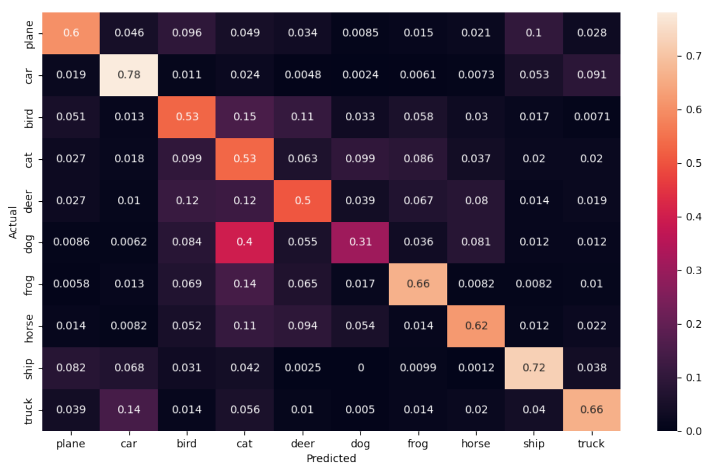
(b) BCNN

Figure 7: Train vs validation accuracy over time

Additionally, neither model converged with the train and validation accuracy, this is an indication that we might need to increase the regularization rate. Another thing to note from figure 7 is that the BCNN took longer to divirge from the train accuracy.



(a) CNN



(b) BCNN

Figure 8: Confusion matrices

The two models have the same set of confusions

5 Closing

References

Fleszar, J. (2023). Bayesian neural networks - capturing the uncertainty of the real world !!

Häse, F., Galván, I. F., Aspuru-Guzik, A., Lindh, R., & Vacher, M. (2019). How machine learning can assist the interpretation of ab initio molecular dynamics simulations and conceptual understanding of chemistry. *Chemical science*, *10*(8), 2298–2307.

Krizhevsky, A., Nair, V., & Hinton, G. (n.d.). Cifar-10 (canadian institute for advanced research). http://www.cs.toronto.edu/~kriz/cifar.html

Saha, S. (2018). A guide to convolutional neural networks — the eli5 way.

Shridhar, K., Laumann, F., & Liwicki, M. (2018). Uncertainty estimations by softplus normalization in bayesian convolutional neural networks with variational inference. *arXiv preprint arXiv:1806.05978*.

Shridhar, K., Laumann, F., & Liwicki, M. (2019). A comprehensive guide to bayesian convolutional neural network with variational inference. *arXiv preprint arXiv:1901.02731*.

What is machine learning (ml)? (2020).

What is machine learning (ml)? (n.d.).