Bayesian Neural Networks

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Neural Networks (NN)
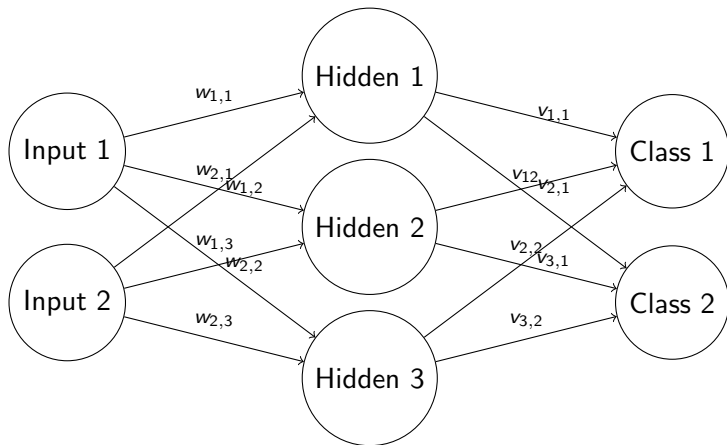

Figure: Example neural network

Issues with Neural Networks

- Stir data and pray
-

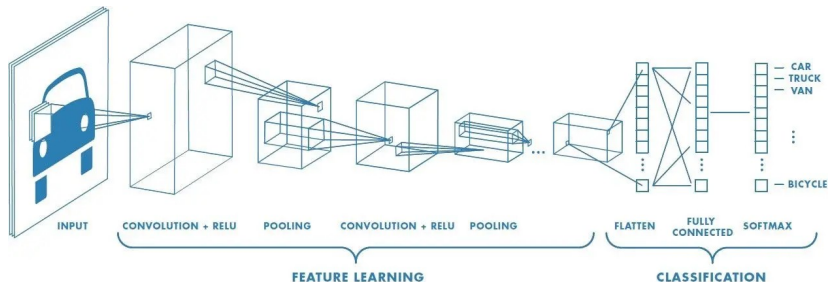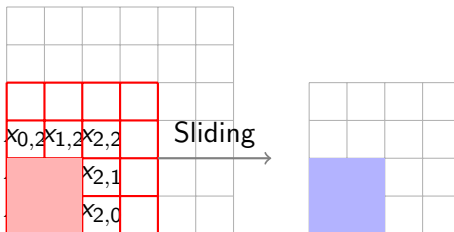Figure: XKCD: "*Machine Learning*" [5]

Convolutional Neural Networks (CNN)

Figure: CNN pipeline [9]

Neural Networks
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Bayesian Neural Networks
○○○○○

Simulation
○○○○○○

Closing
○

References

Convolutional Neural Networks (CNN)

Sliding

$x_{0,2}$ $x_{1,2}$ $x_{2,2}$

$x_{2,1}$

$x_{2,0}$

Convolutional Kernel

Input Matrix

Output Feature Map

Why we use CNNs

Figure: XKCD: "*Self Driving*" [6]

- They are more efficient for image based tasks
- Channels...

Bayesian Neural Network

Figure: Example BNN [1]

Neural Networks
ooooo

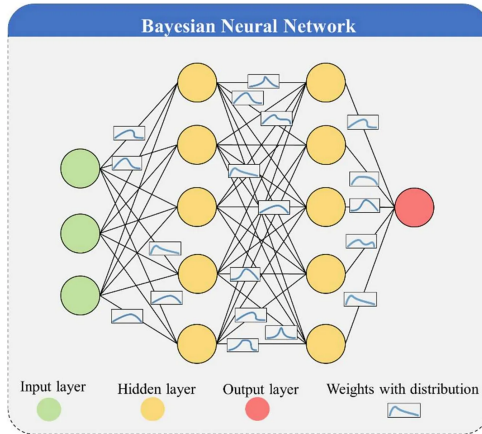Bayesian Neural Networks
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Simulation
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Closing
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References

BNN Neuron
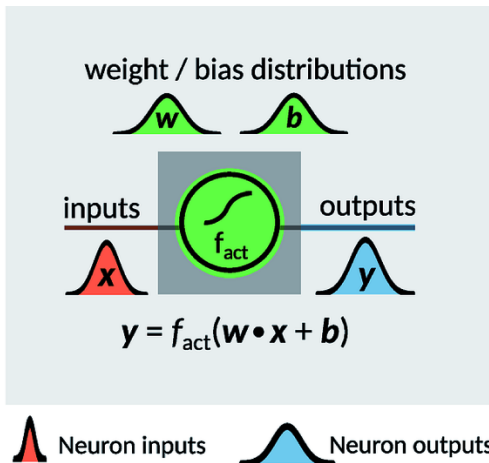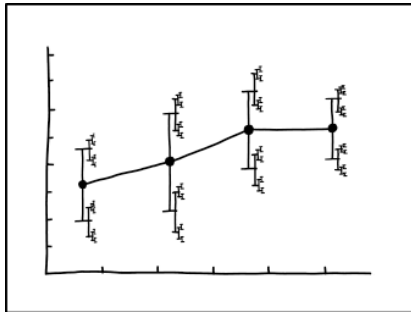

Figure: Example BNN Neuron [2]

Why we use BNN

I DON'T KNOW HOW TO PROPAGATE ERROR CORRECTLY, SO I JUST PUT ERROR BARS ON ALL MY ERROR BARS.

Figure: XKCD: "*Error Bars*" [6]

- We can put uncertainty on our weights

- ....

Applications

Figure: XKCD: "*Simple Answers*" [7]

What are....
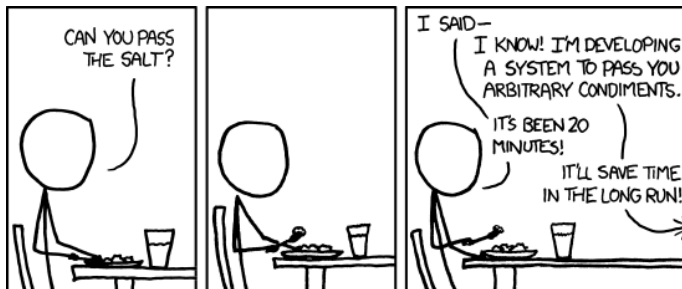
Difference between BNNs and BCNNs

Figure: XKCD: "*The General Problem*" [8]

The relationship between BNNs and BCNNs is the same as NNs and CNNs.

CIFAR-10

airplane

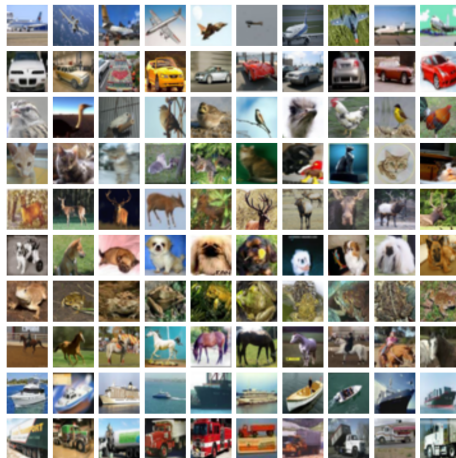automobile

bird

cat

deer

dog

frog

horse

ship

truck

Figure: Example CIFAR-10 images [3]

Hyperparameters

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

Results

Metric	CNN	BCNN
Train Accuracy	81.609%	70.664%
Validation Accuracy	64.499%	61.399%
Time to Train	17 min 6.1 sec	Adamw

Confusion Matrix (CNN)
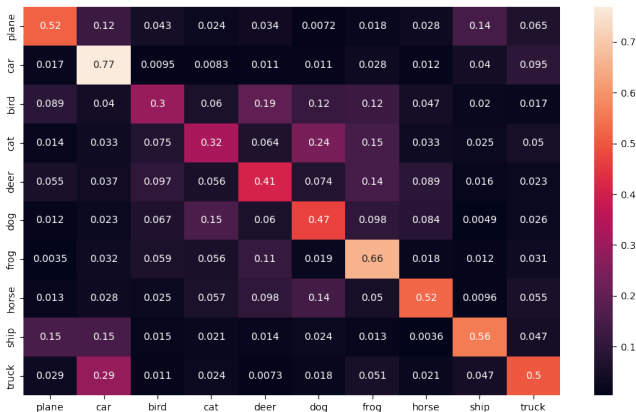
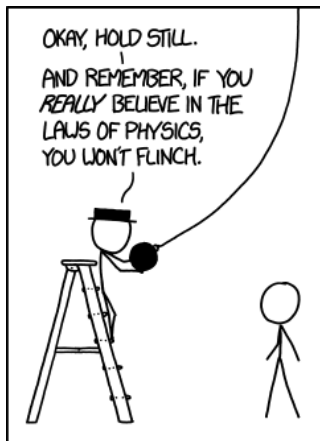# Confusion Matrix (BCNN)
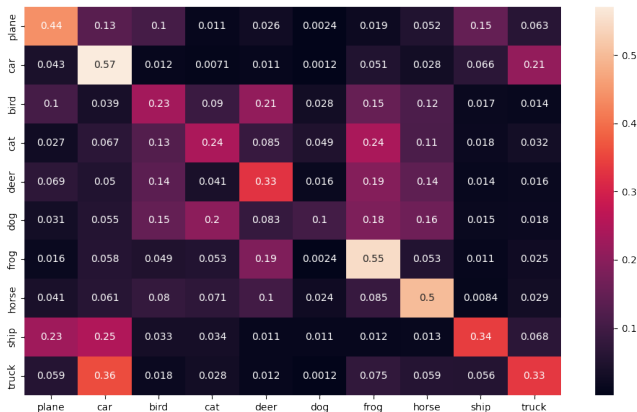
Live Demo

Figure: XKCD: "*Laws of Physics*" [4]

Questions

Figure: XKCD: "*Simple Answers*" [7]

References I

[1]   Jacek Fleszar. "Bayesian Neural Networks - Capturing The
      Uncertainty Of The Real World !!" In: (Sept. 2023).

[2]   Florian Häse et al. "How machine learning can assist the
      interpretation of ab initio molecular dynamics simulations and
      conceptual understanding of chemistry". In: *Chemical science* 10.8
      (2019), pp. 2298–2307.

[3]   Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. "CIFAR-10
      (Canadian Institute for Advanced Research)". In: (). URL:
      http://www.cs.toronto.edu/~kriz/cifar.html.

[4]   Randall Monroe. *XKCD: Laws of Physics*. Apr. 2016.

[5]   Randall Monroe. *XKCD: Machine Learning*. May 2017.

[6]   Randall Monroe. *XKCD: Self Driving*. Oct. 2017.

References II

[7]   Randall Monroe. *XKCD: Simple Answers*. Nov. 2013.

[8]   Randall Monroe. *XKCD: The General Problem*. Nov. 2011.

[9]   Sumit Saha. "A Guide to Convolutional Neural Networks — the ELI5 way". In: (Dec. 2018).