

Bayesian Neural Networks

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Neural Networks (NN)

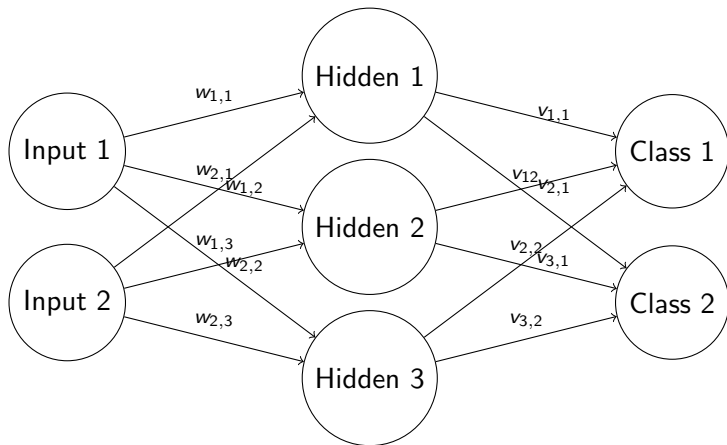


Figure: Example neural network



A Neural Network Neuron

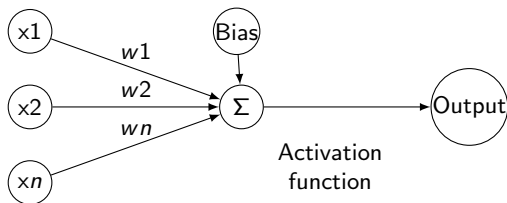


Figure: Example neural network neuron



Issues with Neural Networks

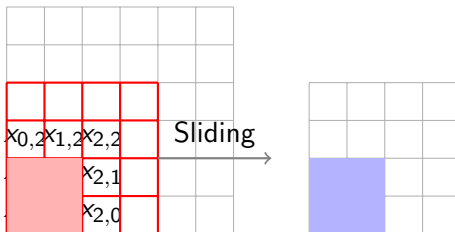


- Stir data and pray
- Interpretability problems
- Lots of data required
- Risk of overfitting
- Unpredictable failures to generalize
- No uncertainty quantification
- Computationally expensive



Figure: XKCD: "Machine Learning" [5]

Convolutional Neural Networks (CNN)



Convolutional Kernel Input Matrix

Output Feature Map



Convolutional Neural Networks (CNN)

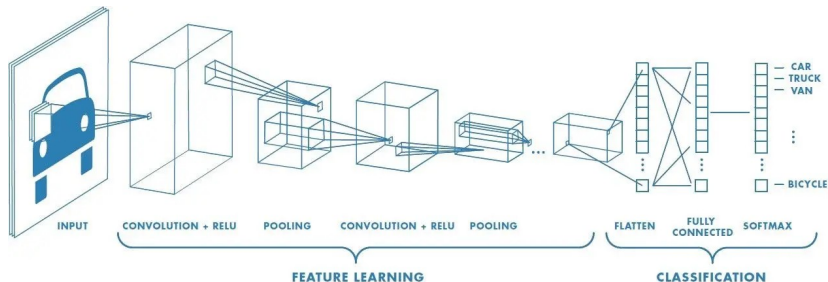


Figure: CNN pipeline [9]



Why we use CNNs



SO MUCH OF "AI" IS JUST FIGURING OUT WAYS TO OFFLOAD WORK ONTO RANDOM STRANGERS.

- Fewer parameters
- Encode spatial patterns
- More efficient for image tasks

Figure: XKCD: "Self Driving" [6]



Bayesian Neural Network

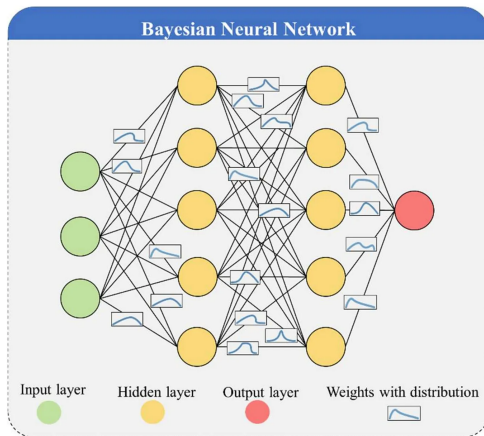


Figure: Example BNN [1]



BNN Neuron

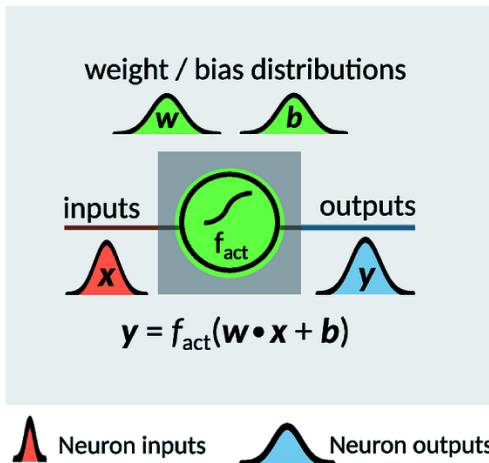
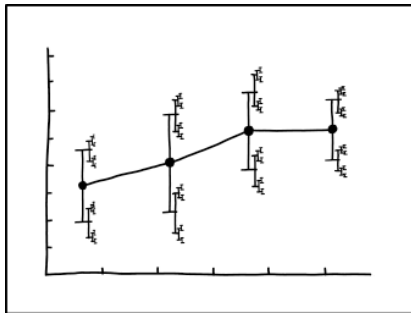


Figure: Example BNN Neuron [2]



Why we use BNN



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

- Well-calibrated uncertainty
- Handles sparse data while minimizing overfitting
- More predictable failures
- Formalizes prior knowledge and assumptions
- Inherent sequentiality

Figure: XKCD: "Error Bars" [6]



Applications

THE
SIMPLE ANSWERS
TO THE QUESTIONS THAT GET ASKED
ABOUT EVERY NEW TECHNOLOGY:

WILL <input type="checkbox"/> MAKE US ALL GENIUSES?	NO
WILL <input type="checkbox"/> MAKE US ALL MORONS?	NO
WILL <input type="checkbox"/> DESTROY WHOLE INDUSTRIES?	YES
WILL <input type="checkbox"/> MAKE US MORE EMPATHETIC?	NO
WILL <input type="checkbox"/> MAKE US LESS CARING?	NO
WILL TEENS USE <input type="checkbox"/> FOR SEX?	YES
WERE THEY GOING TO HAVE SEX ANYWAY?	YES
WILL <input type="checkbox"/> DESTROY MUSIC?	NO
WILL <input type="checkbox"/> DESTROY ART?	NO
BUT CAN'T WE GO BACK TO A TIME WHEN--	NO
WILL <input type="checkbox"/> BRING ABOUT WORLD PEACE?	NO
WILL <input type="checkbox"/> CAUSE WIDESPREAD ALIENATION BY CREATING A WORLD OF EMPTY EXPERIENCES?	WE WERE ALREADY ALIENATED

- Uncertainty quantification
 - Engineering, Medicine, Finance, ...
- Sparse data
 - Anywhere data is expensive
 - Medical diagnosis
 - Molecular biology
- Warnings before failing to generalize
 - Autonomous driving
 - Engineering
- Sequentiality



Figure: XKCD: "Simple Answers" [7]

Difference between BNNs and BCNNs

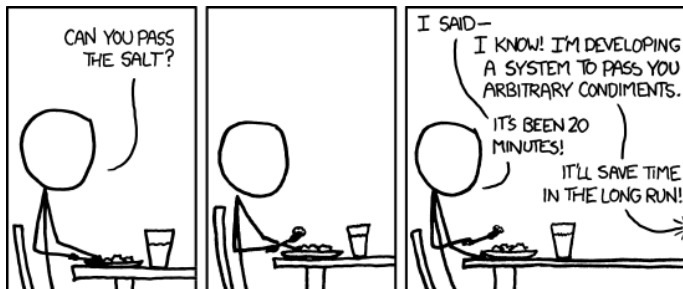


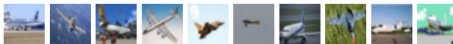
Figure: XKCD: "The General Problem" [8]

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



CIFAR-10

airplane



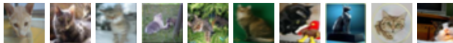
automobile



bird



cat



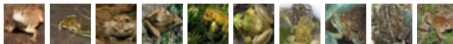
deer



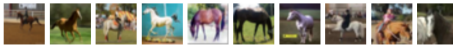
dog



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

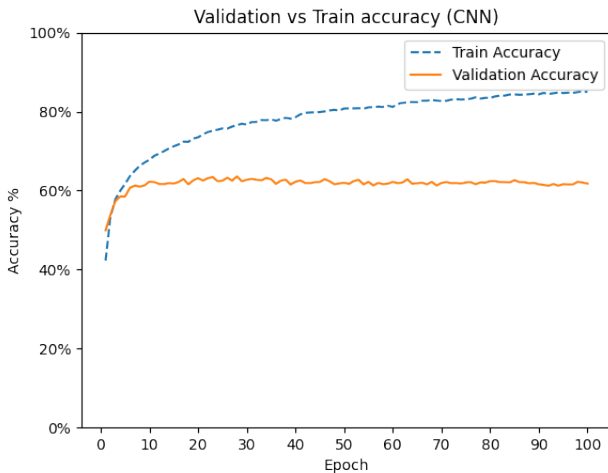


Results

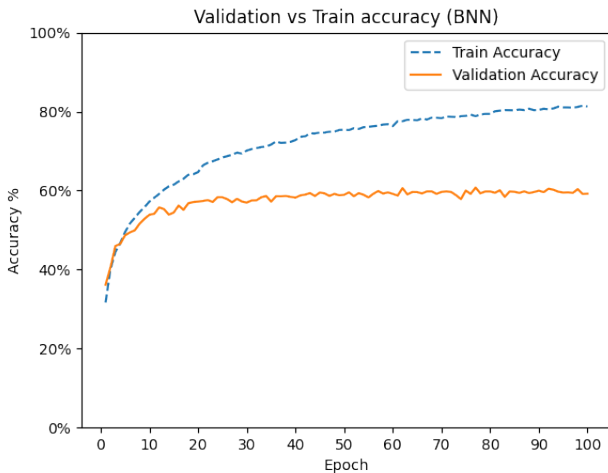
Metric	CNN	BCNN
Train Accuracy	84.96%	81.27%
Validation Accuracy	61.76%	59.21%
Time to Train	16 min 11 sec	22 min 11 sec



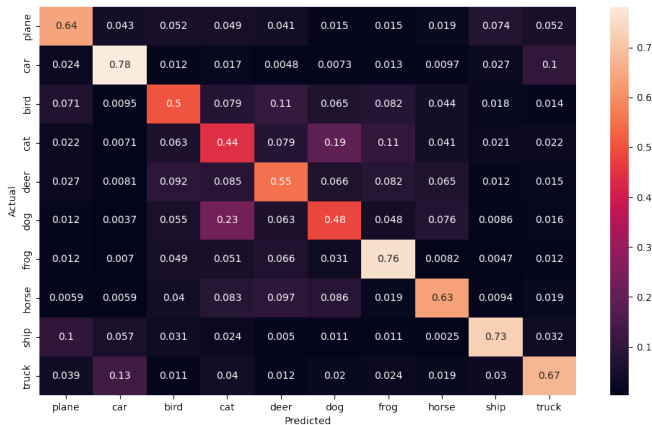
Accuracy over time (CNN)



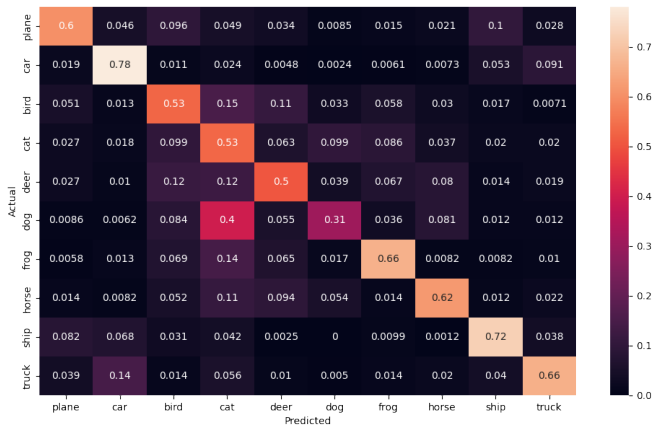
Accuracy over time (BNN)



Confusion Matrix (CNN)



Confusion Matrix (BCNN)



Live Demo

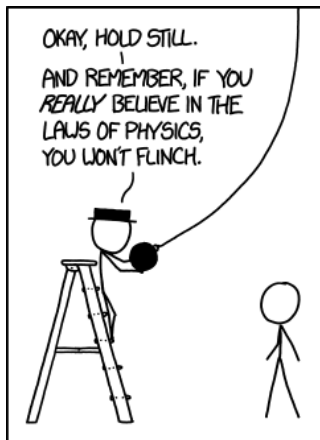


Figure: XKCD: "Laws of Physics" [4]



Questions

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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).

