Bayesian Neural Networks

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April 23, 2024

Neural Networks (NN)

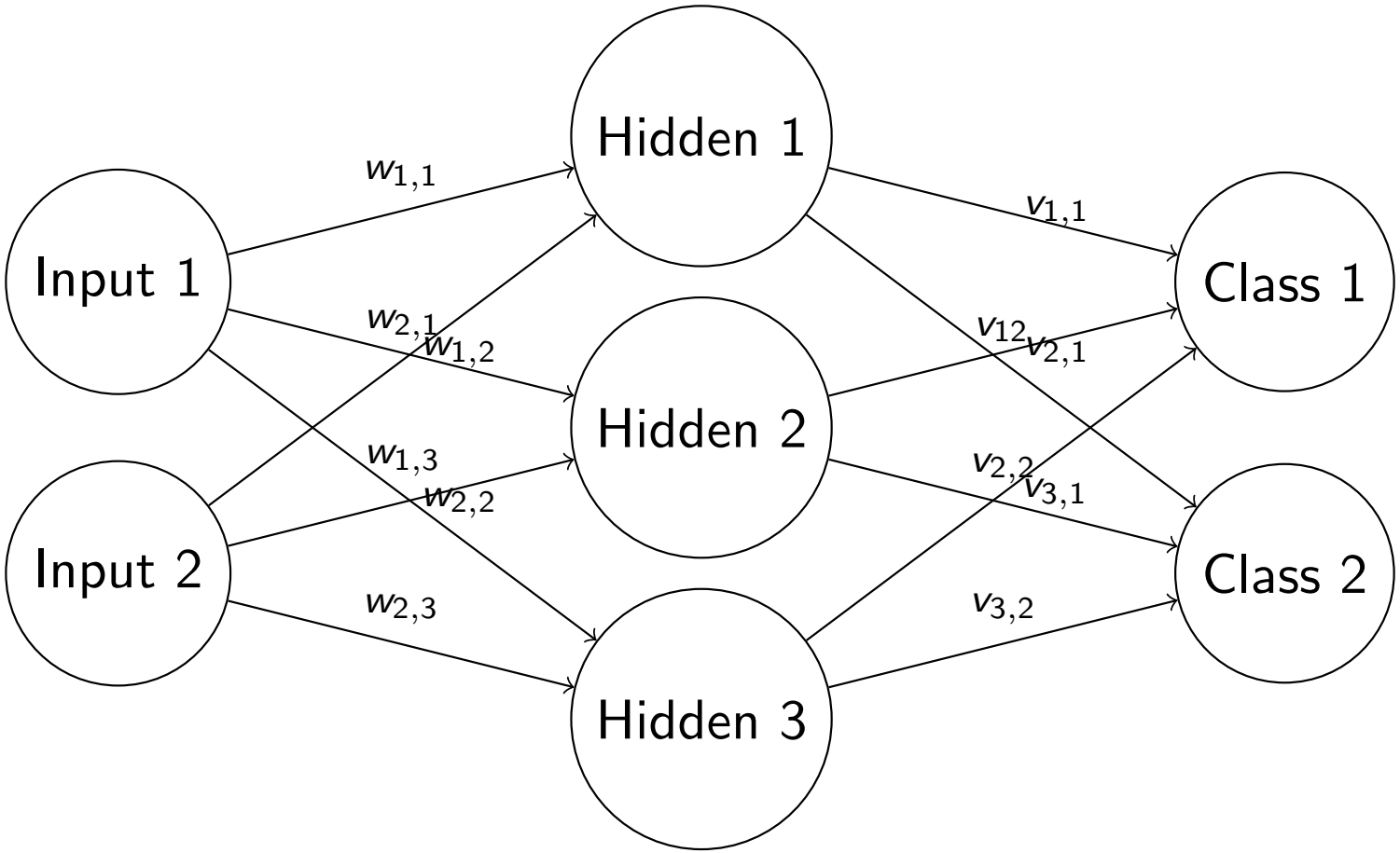


Figure: Example neural network

A Neural Network Neuron

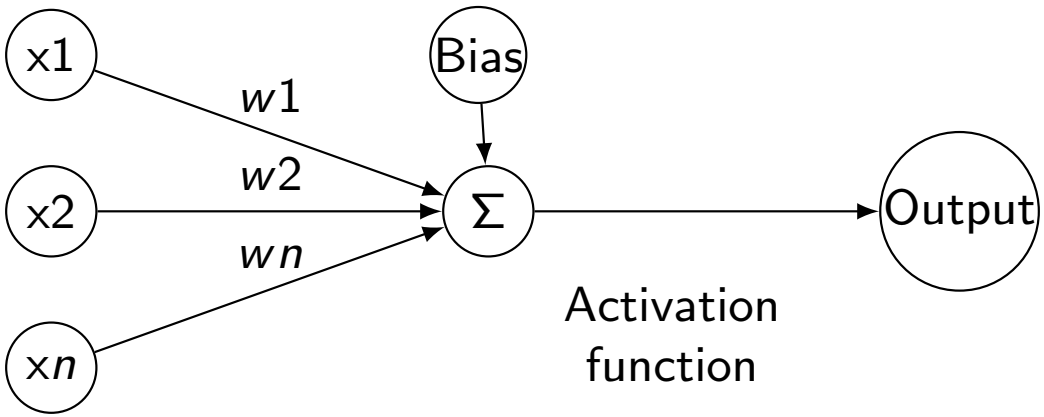


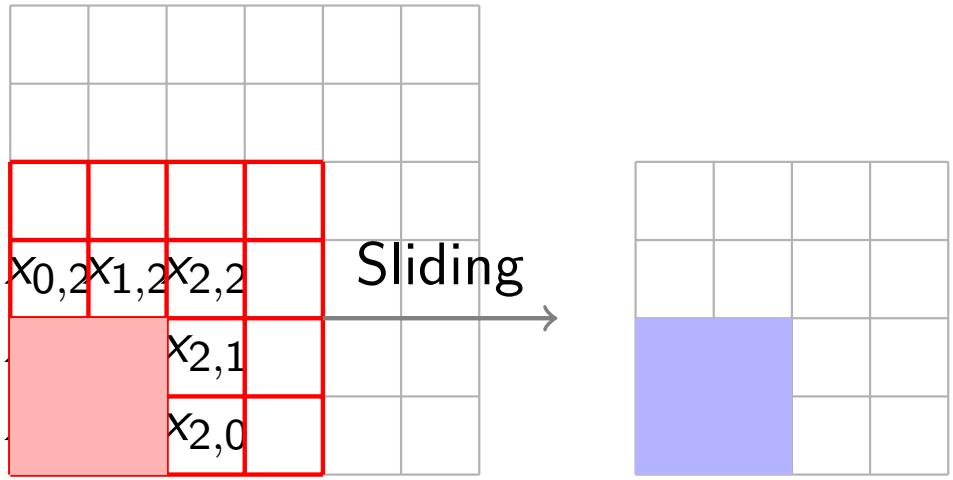
Figure: Example neural network neuron

Issues with Neural Networks

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

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

Convolutional Neural Networks (CNN)



Convolutional Kernel

Input Matrix

Output Feature Map

Convolutional Neural Networks (CNN)

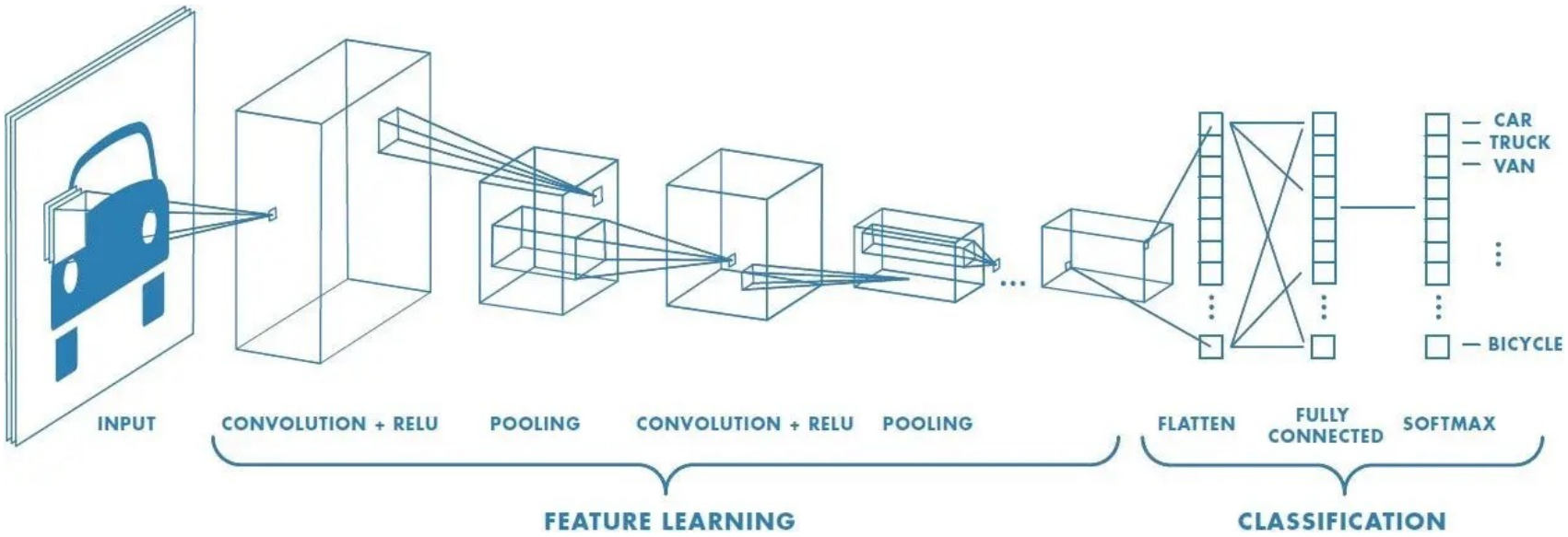


Figure: CNN pipeline [9]

Why we use CNNs

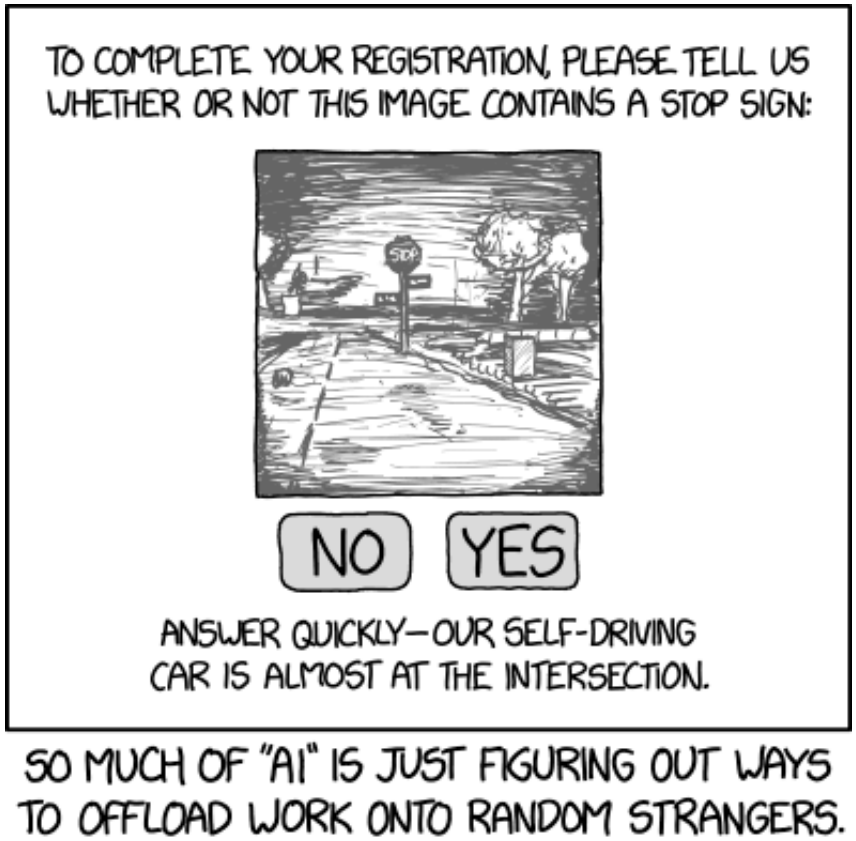


Figure: XKCD: "*Self Driving*" [6]

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

Bayesian Neural Network

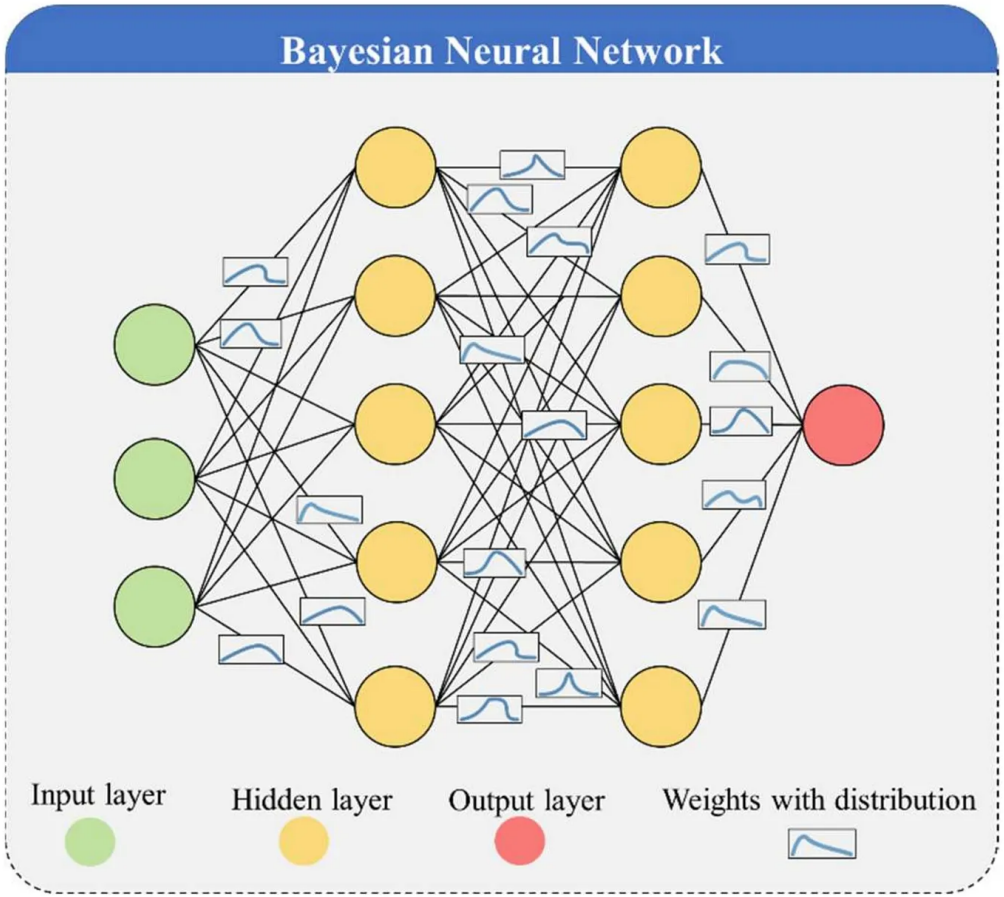


Figure: Example BNN [1]

BNN Neuron

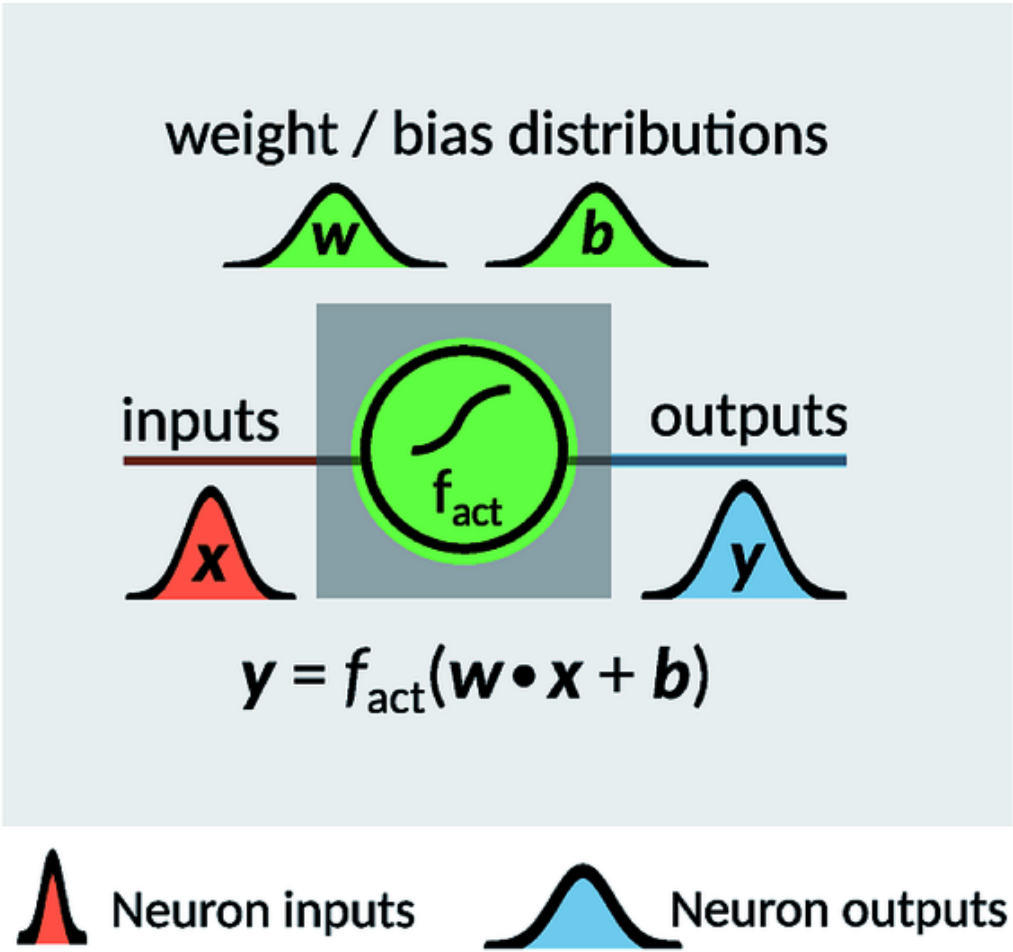


Figure: Example BNN Neuron [2]

Why we use BNN

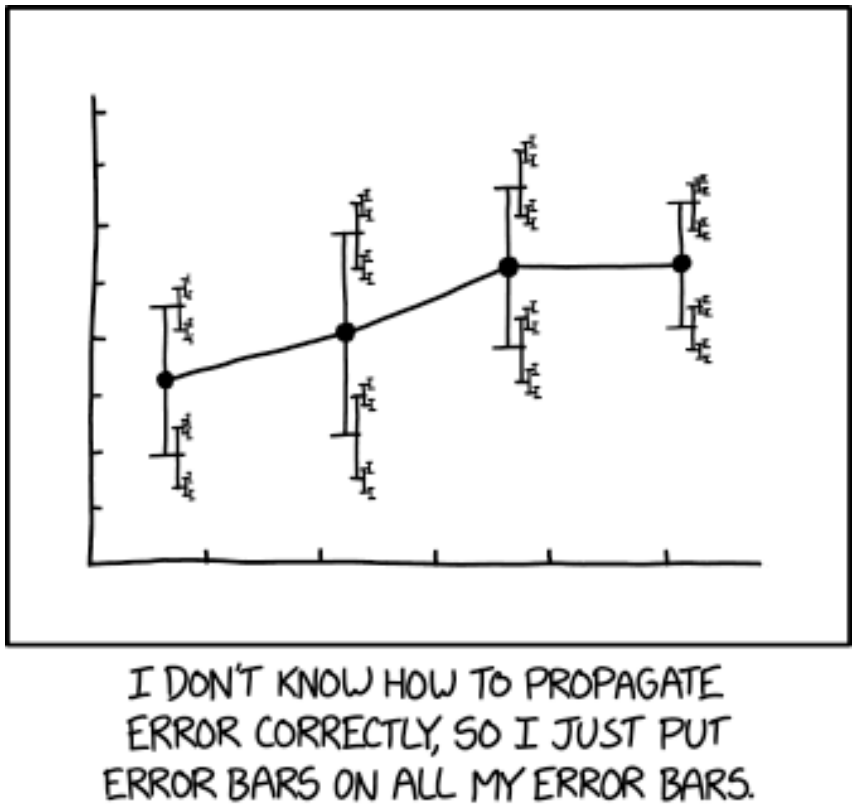


Figure: XKCD: "*Error Bars*" [6]

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

Applications

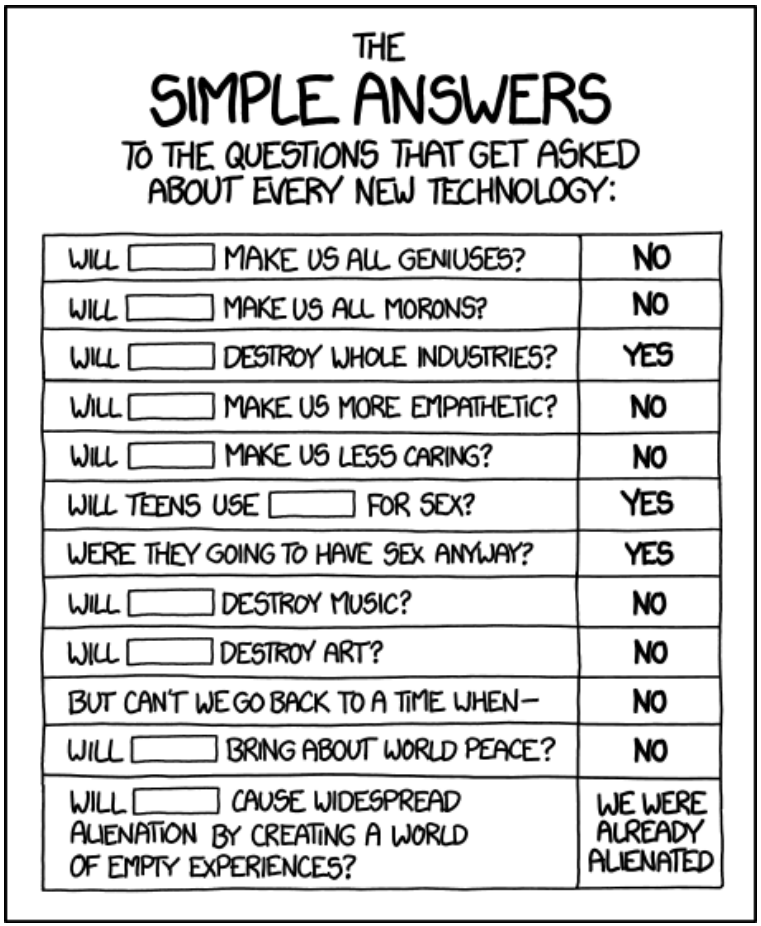


Figure: XKCD: "*Simple Answers*" [7]

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

Difference between BNNs and BCNNs

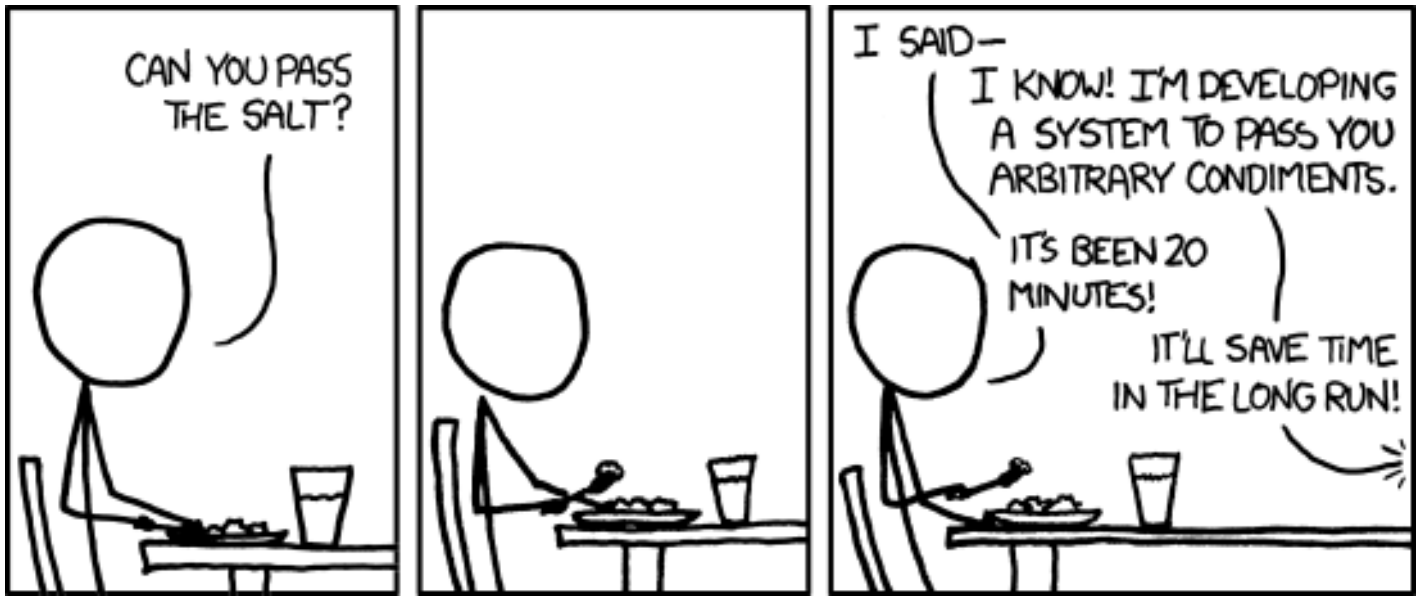


Figure: XKCD: "*The General Problem*" [8]

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

CIFAR-10

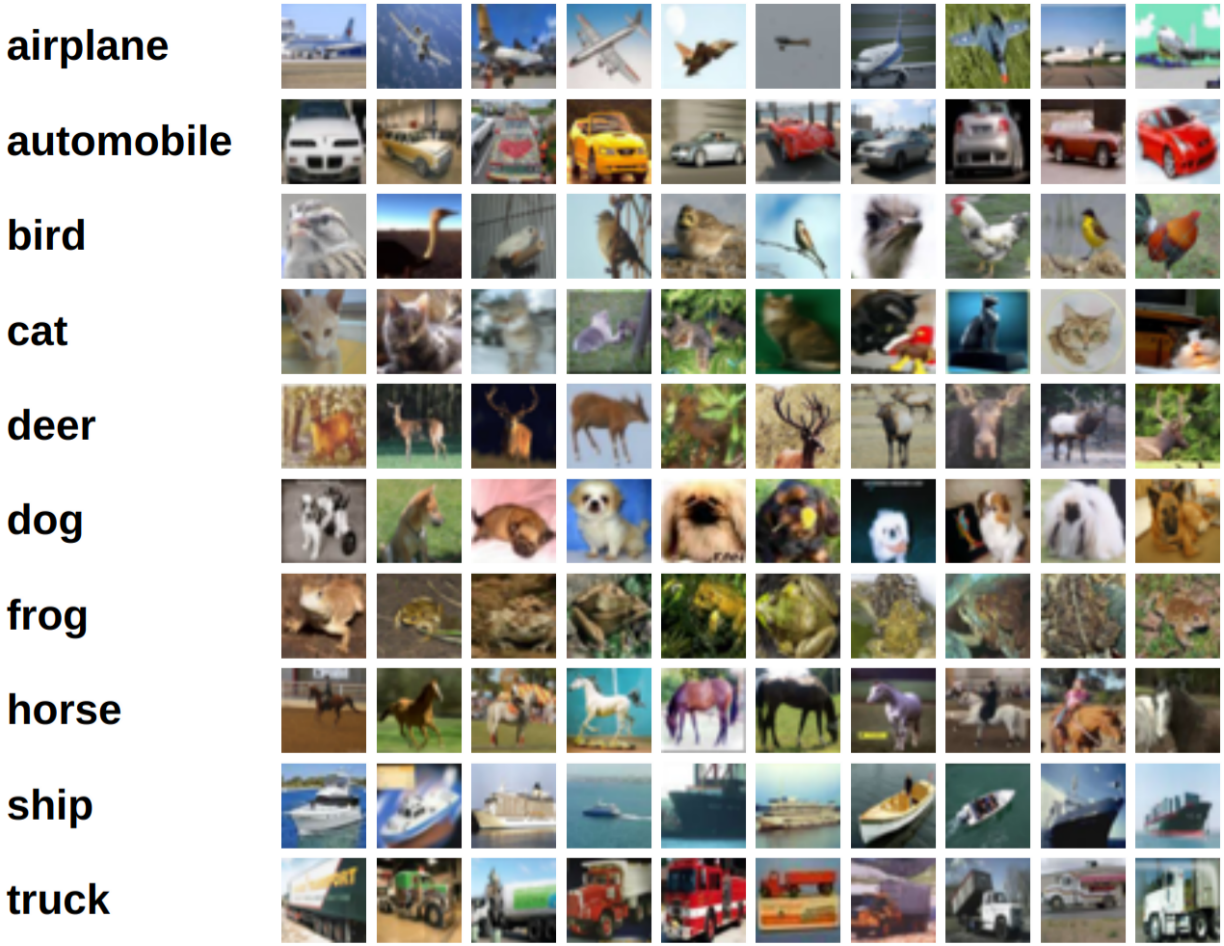


Figure: Example CIFAR-10 images [3]

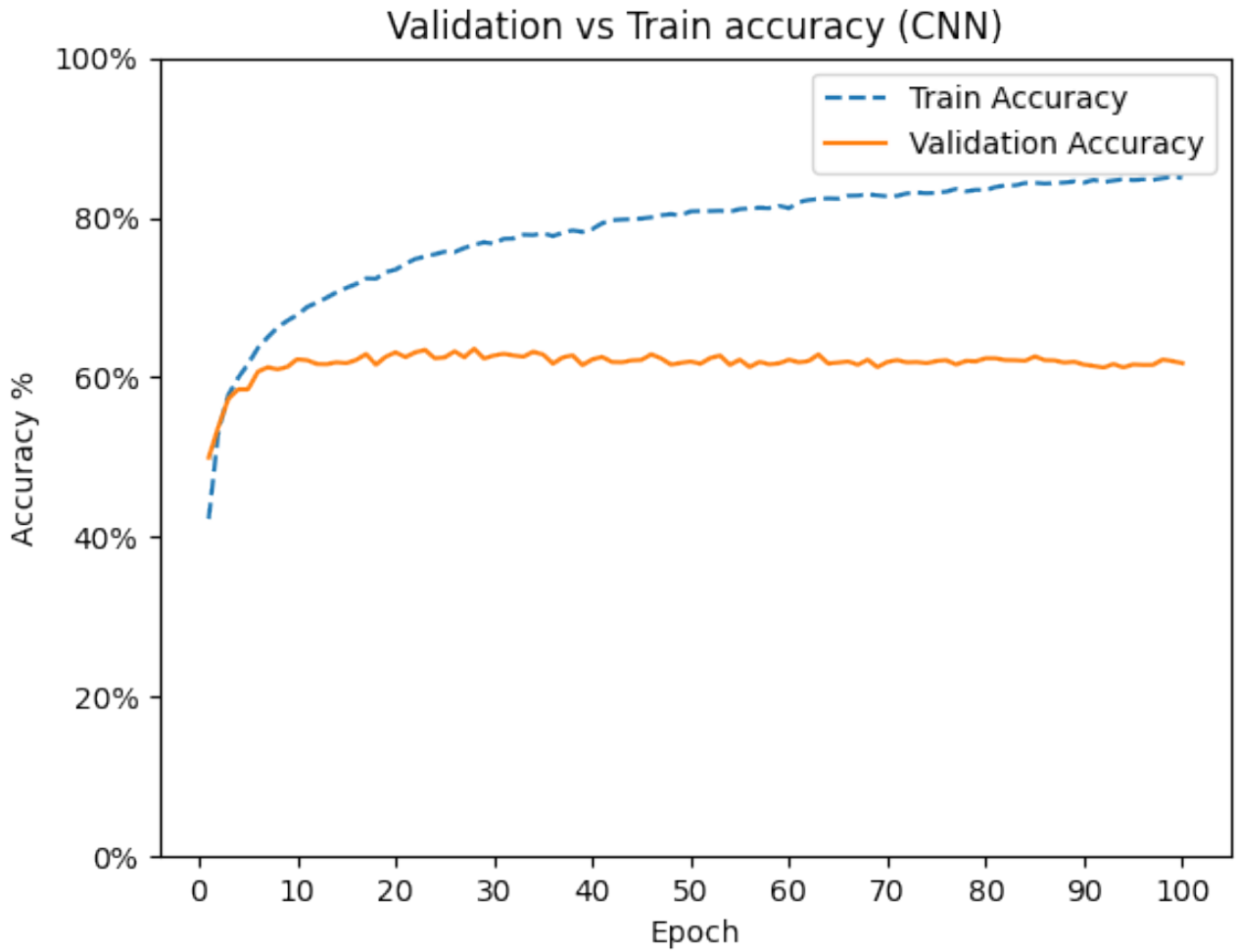
Hyperparameters

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

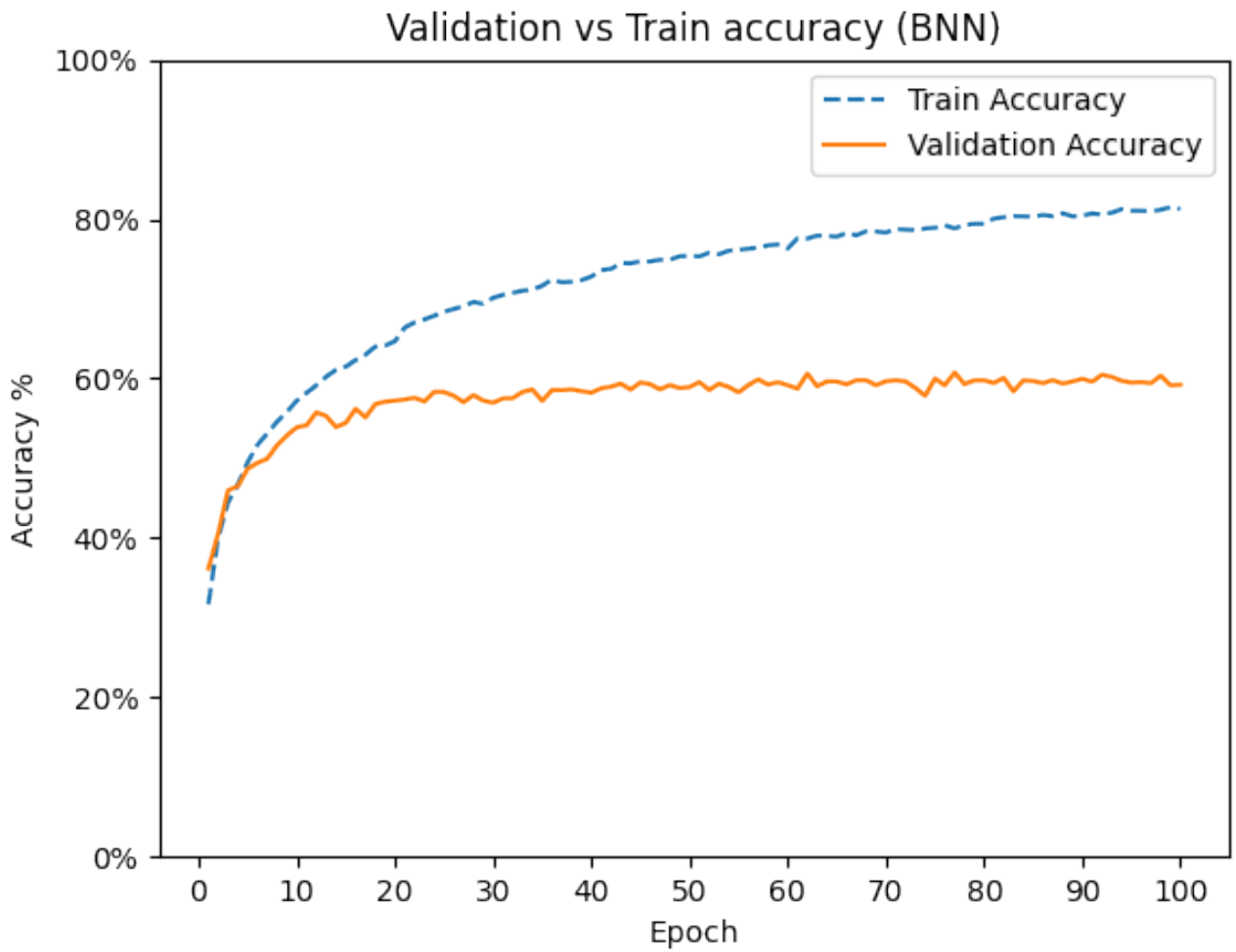
Results

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

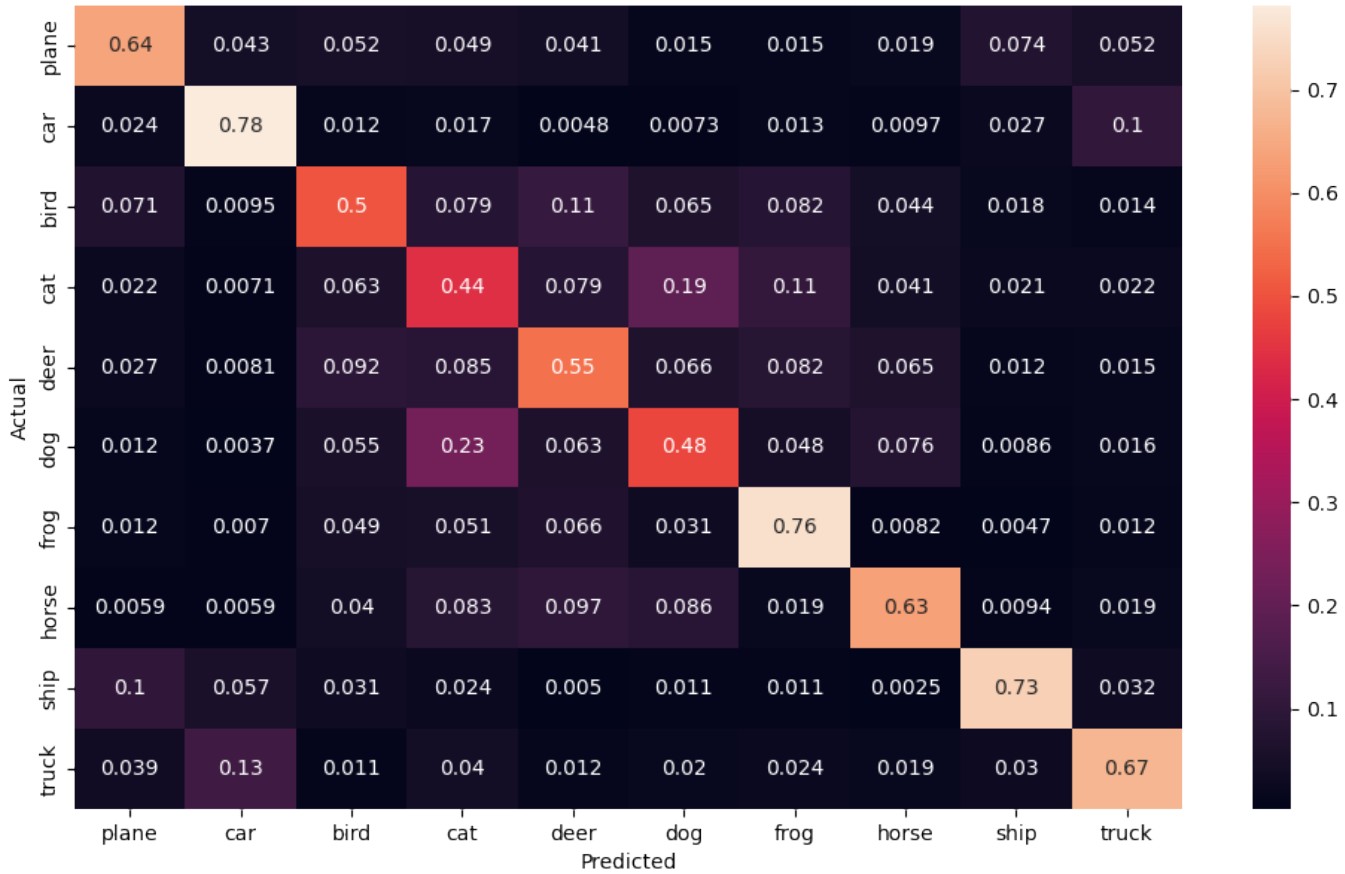
Accuracy over time (CNN)



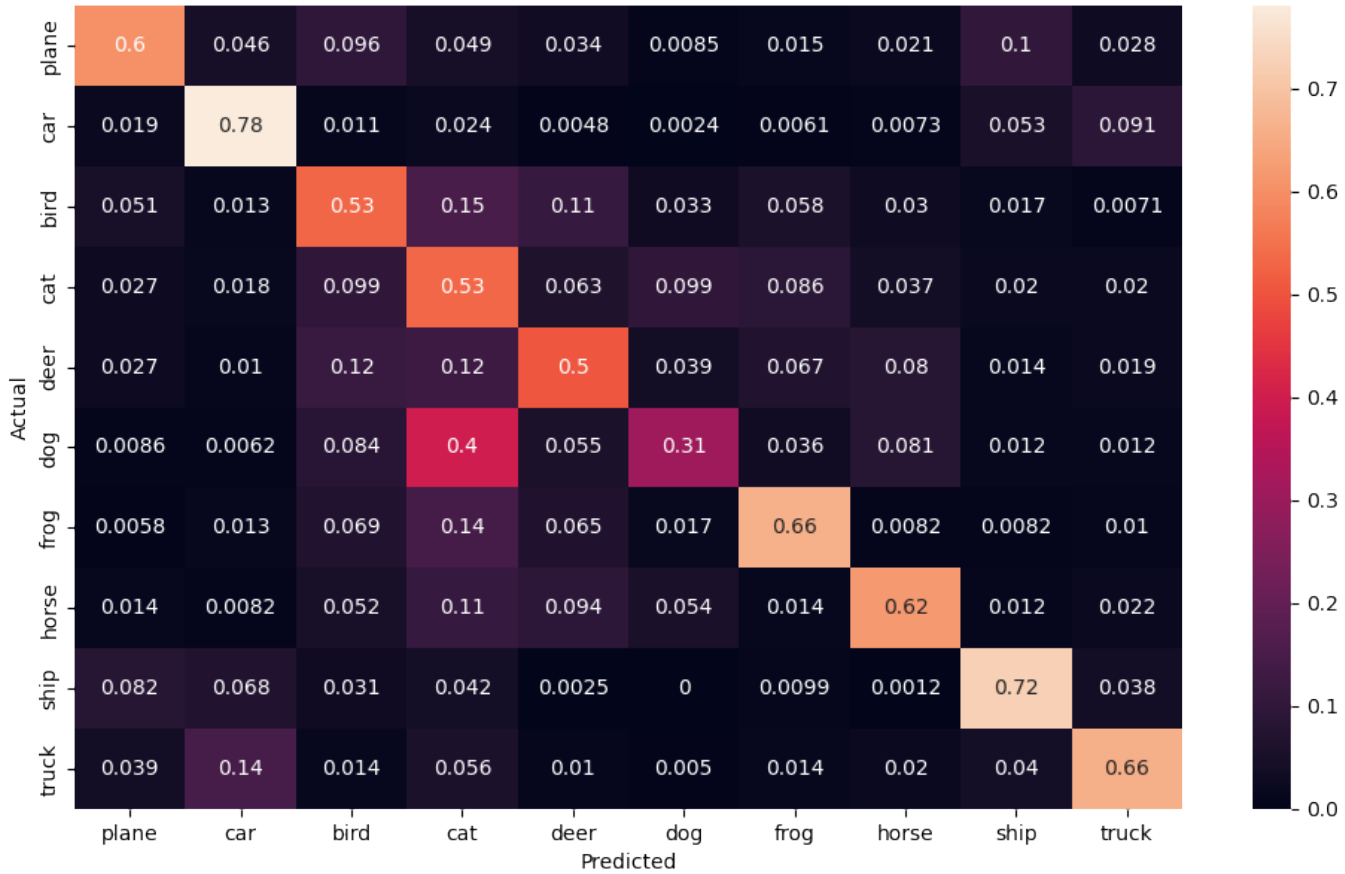
Accuracy over time (BNN)



Confusion Matrix (CNN)



Confusion Matrix (BCNN)



Live Demo

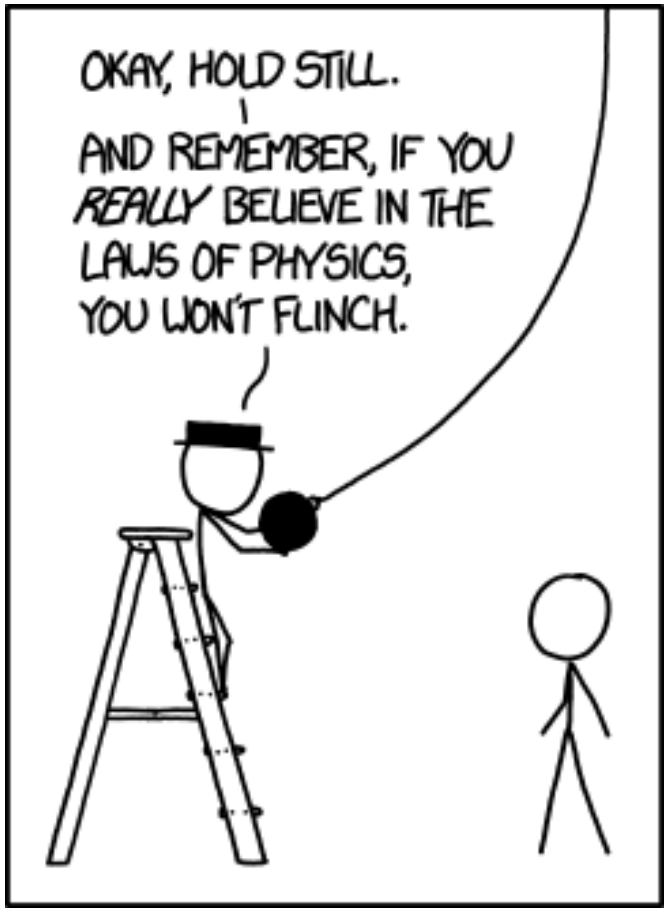


Figure: XKCD: "*Laws of Physics*" [4]

Questions

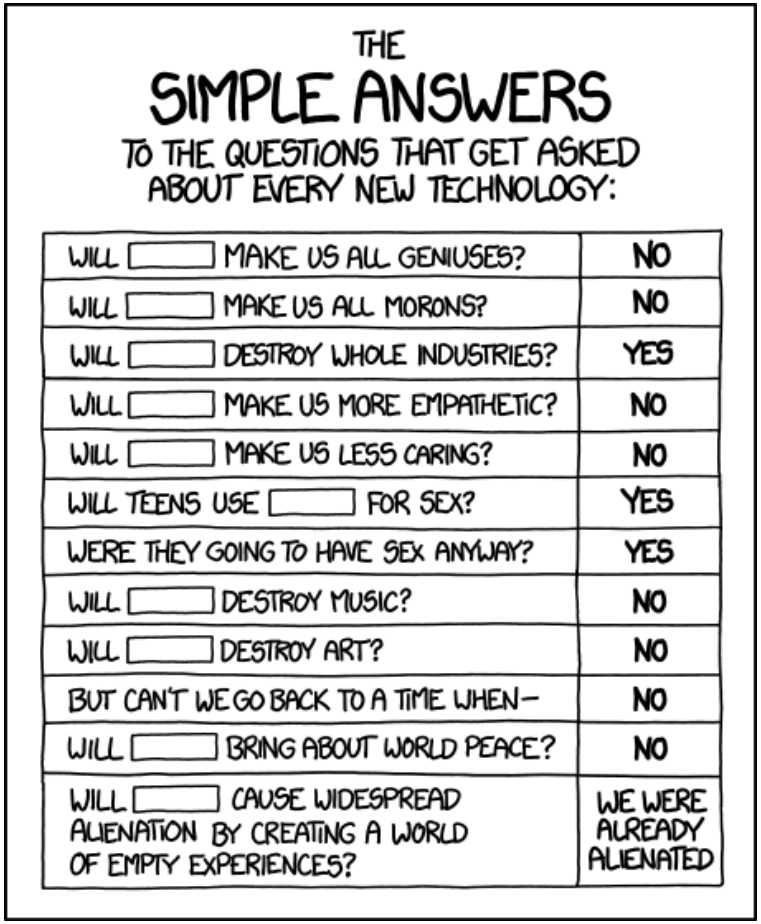


Figure: XKCD: "*Simple Answers*" [7]

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).