Research and development to speed up machine learning by using a quantum computer
量子コンピュータを使った機械学習の高速化の研究開発

Philip Carr

Outline

- Introduction
- Background
- Machine Learning
  - Previous Research
  - Dense Neural Networks, Restricted Boltzmann Machines, and Deep Belief Networks
- Implementation
- Results
- Conclusion and Future Developments

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  - Quantum computing, which offers an entirely new way to perform computational tasks by directly making use of the behavior of quantum mechanical systems, allowing for the efficient computation of many problems intractable for classical computers
- The question now is: Can quantum computing be used to advance the potential of machine learning?

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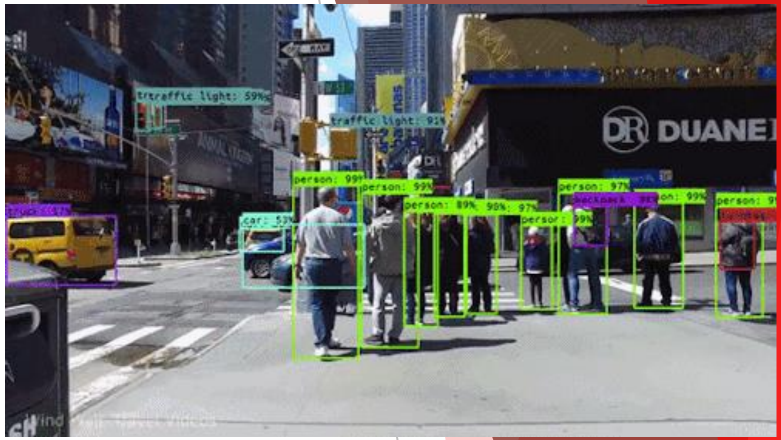

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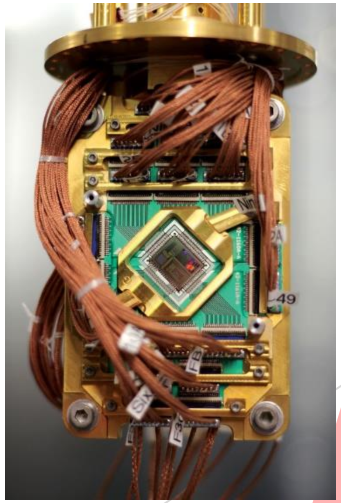

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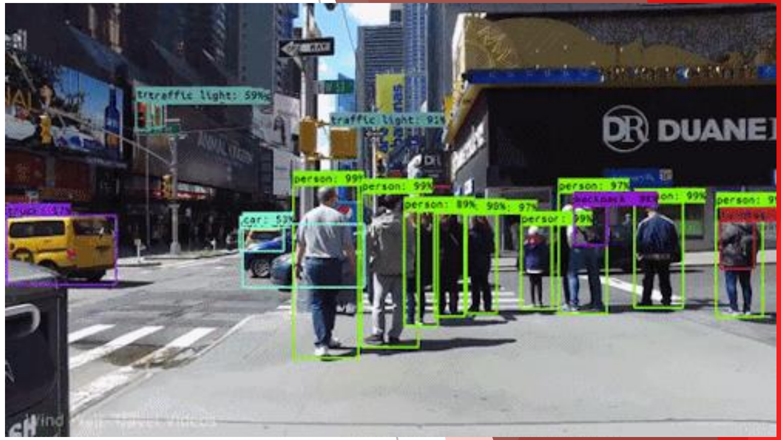

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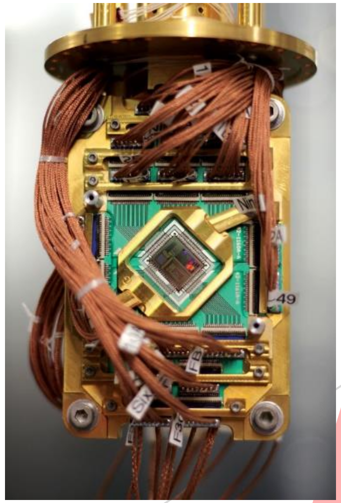

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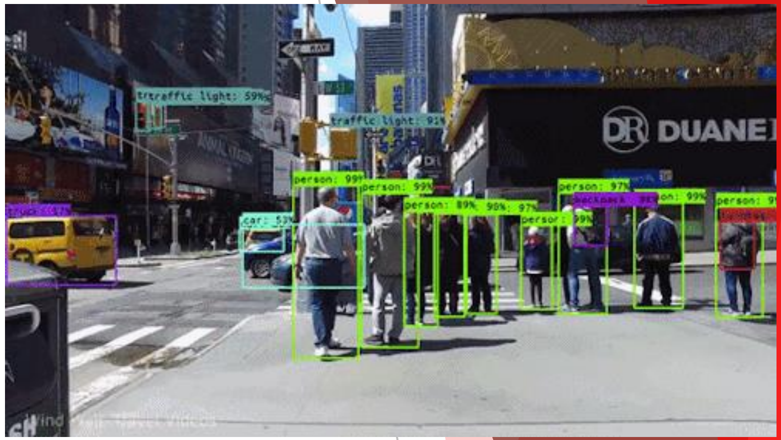

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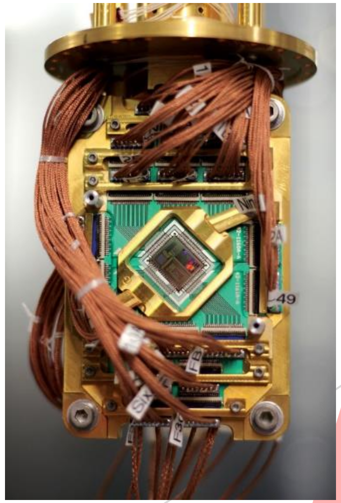

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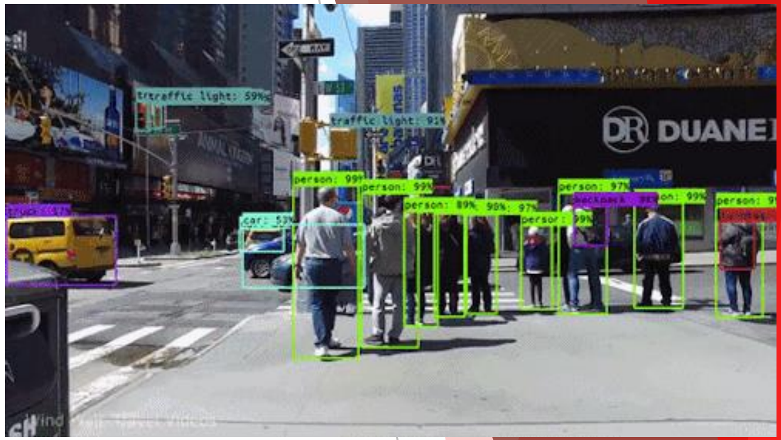

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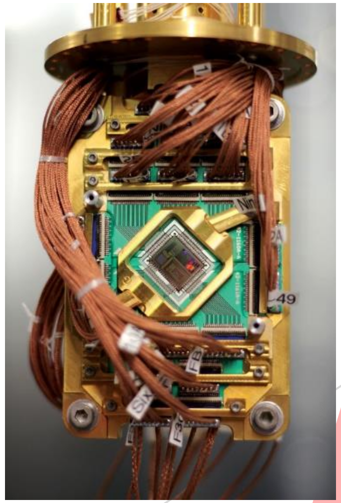

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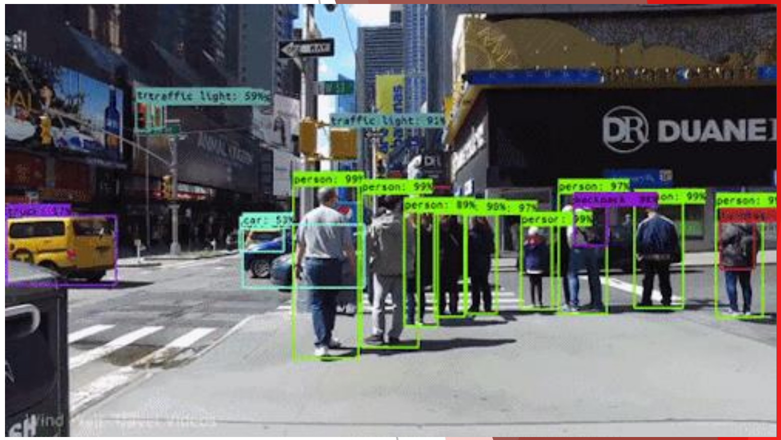

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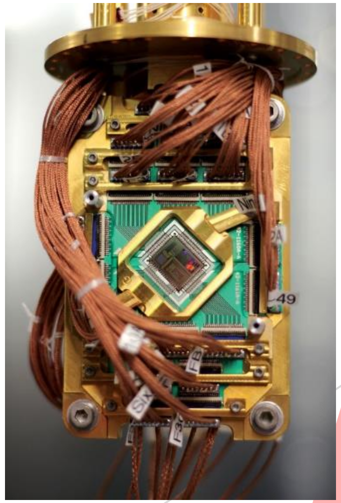

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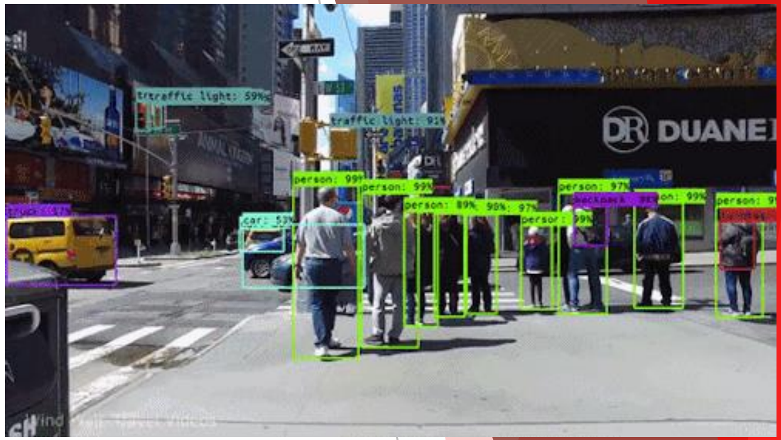

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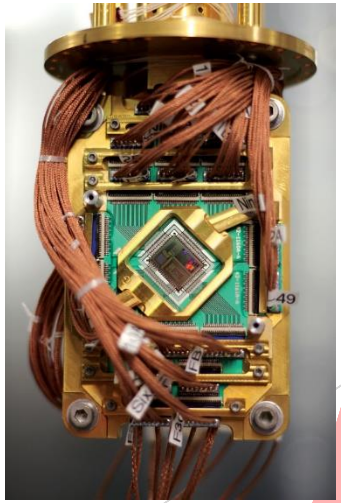

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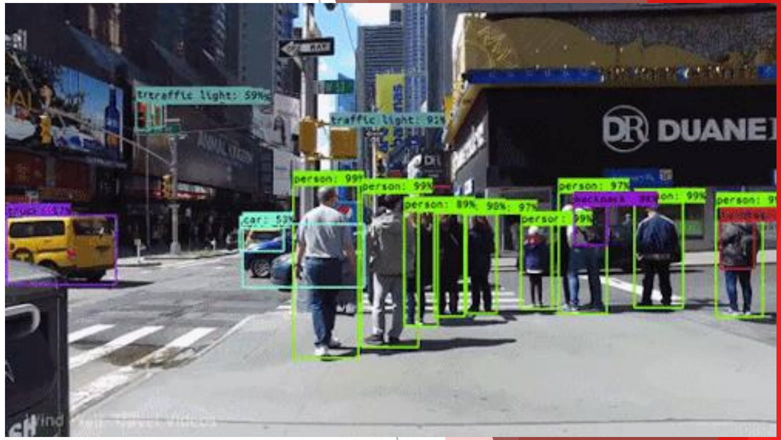

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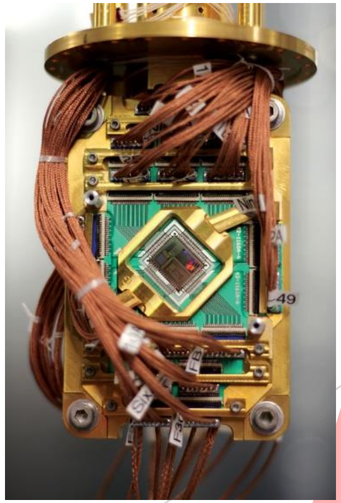

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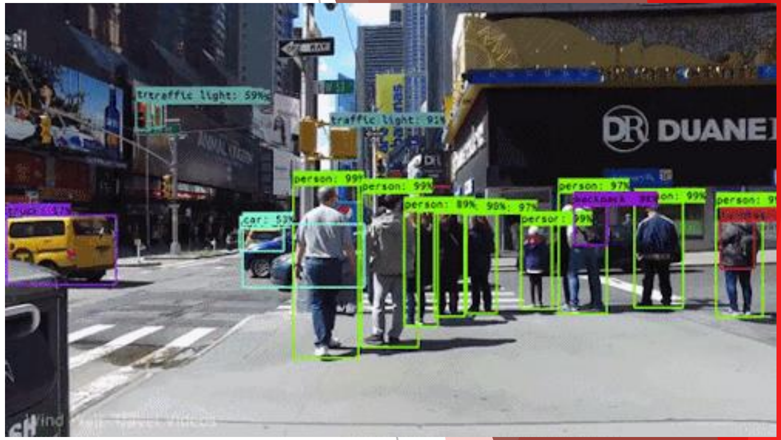

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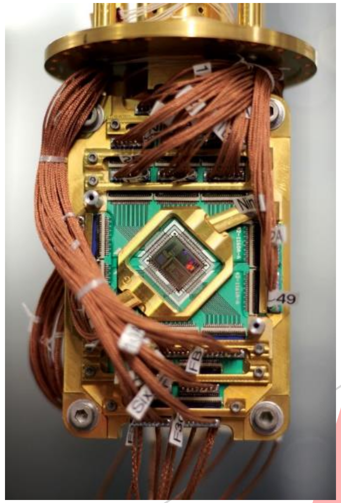

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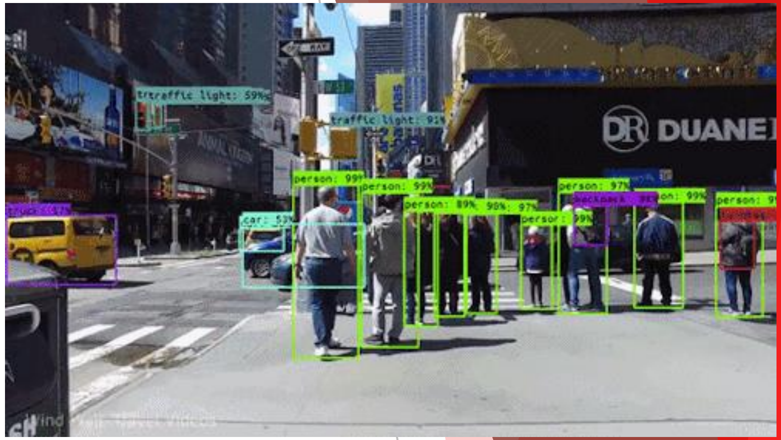

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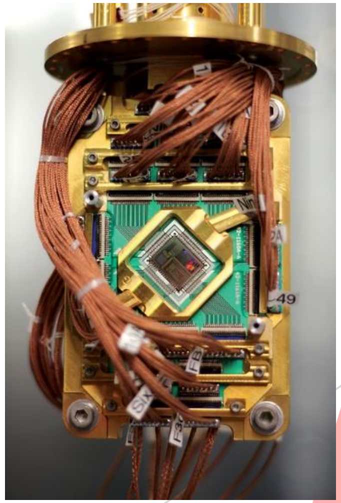

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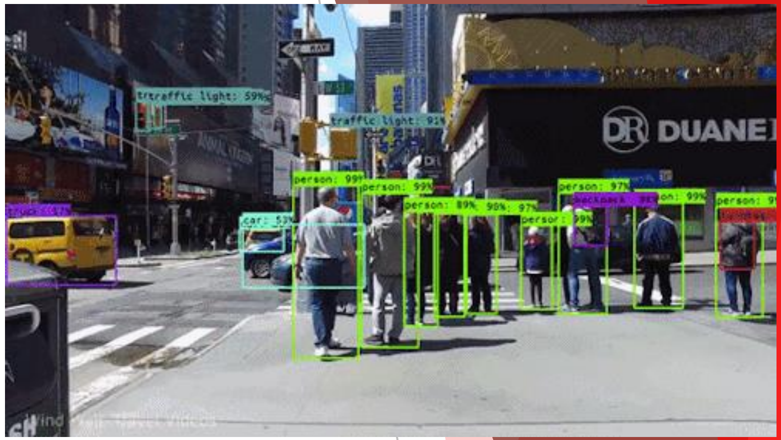

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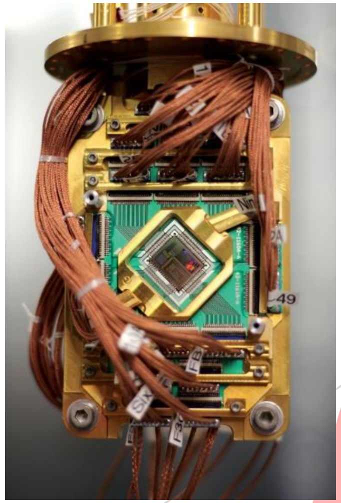

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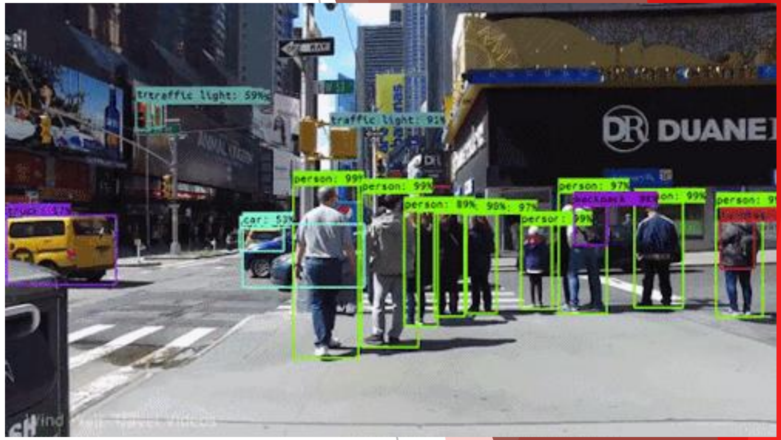

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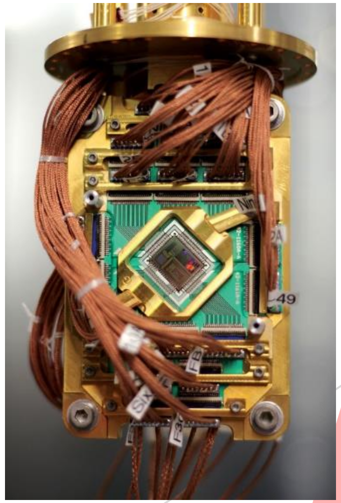

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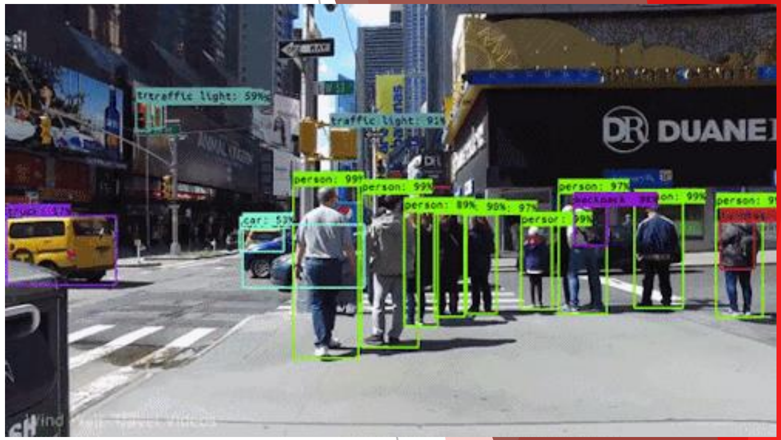

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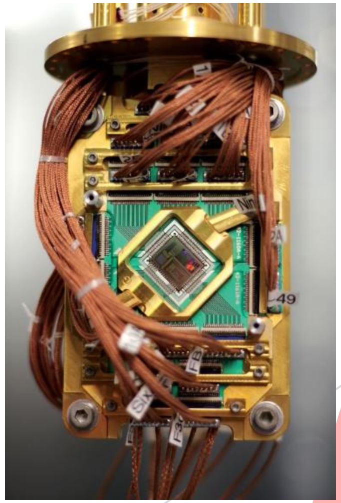

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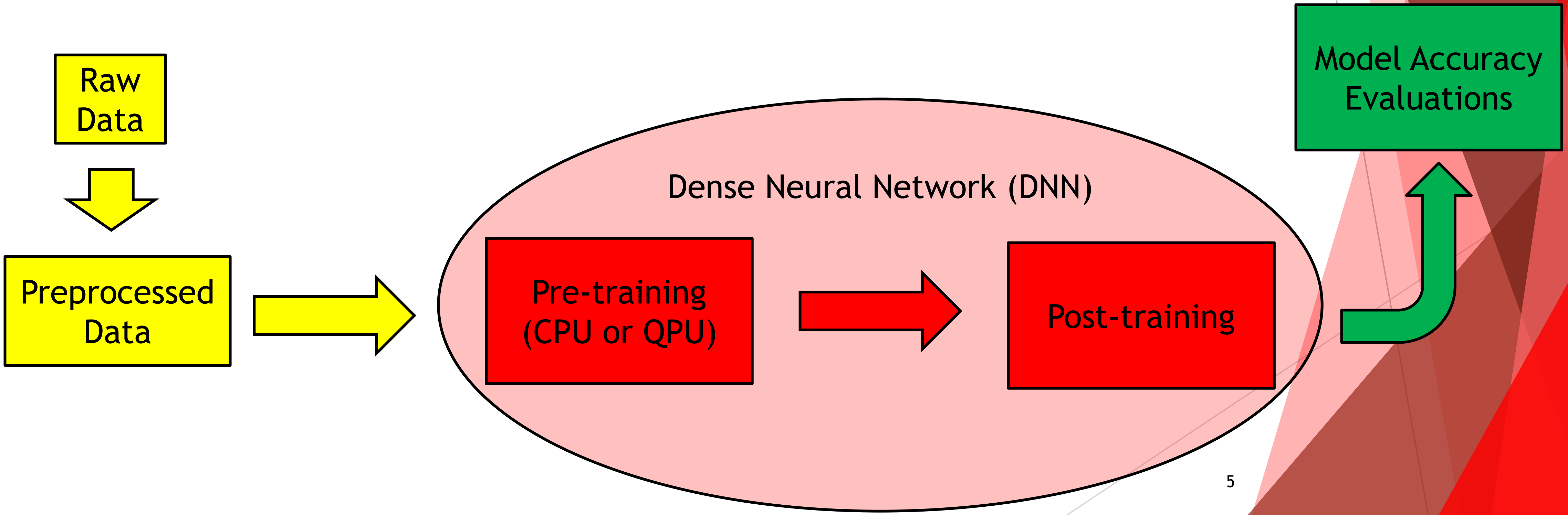

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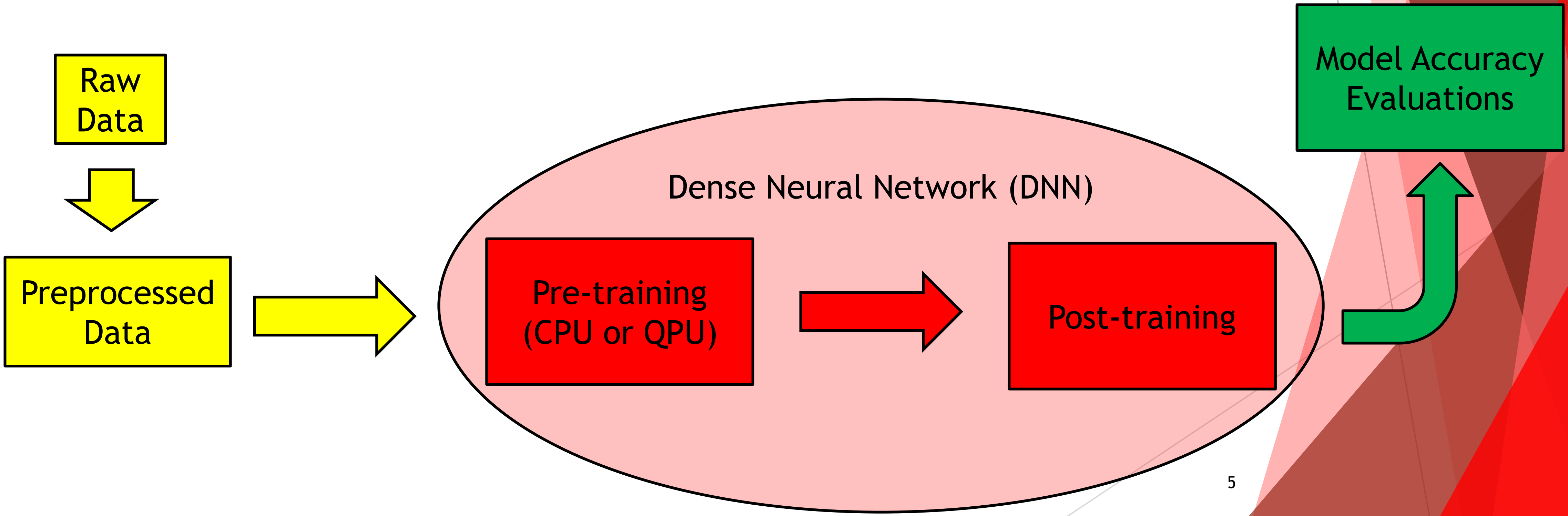

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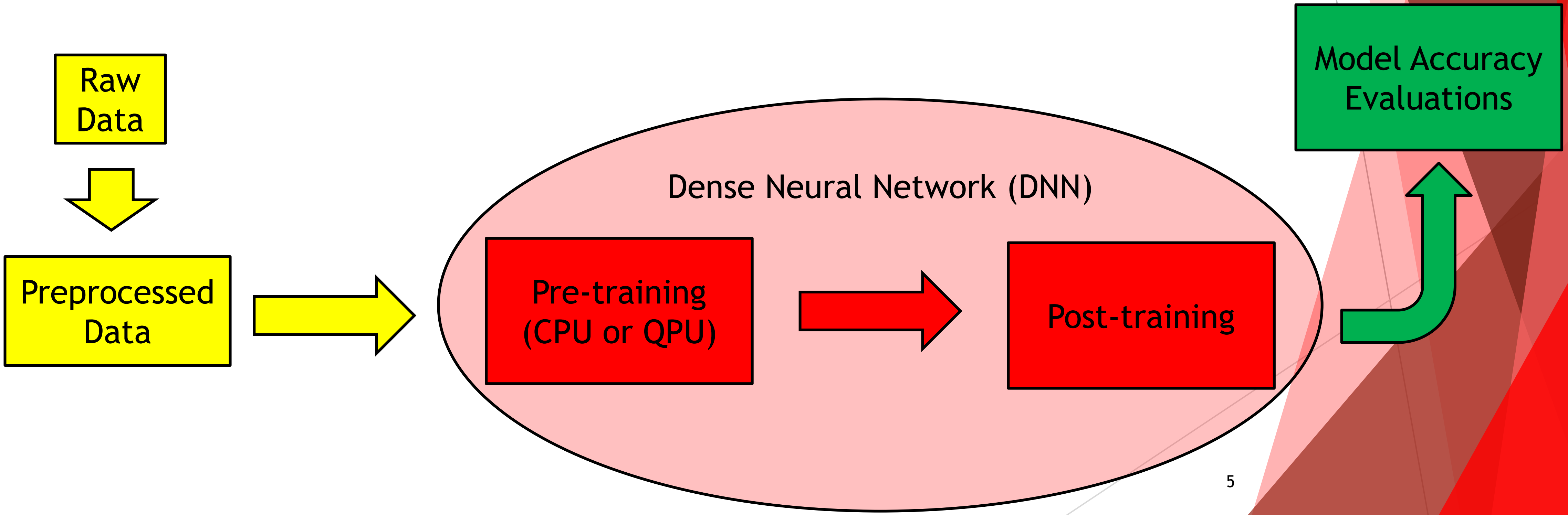

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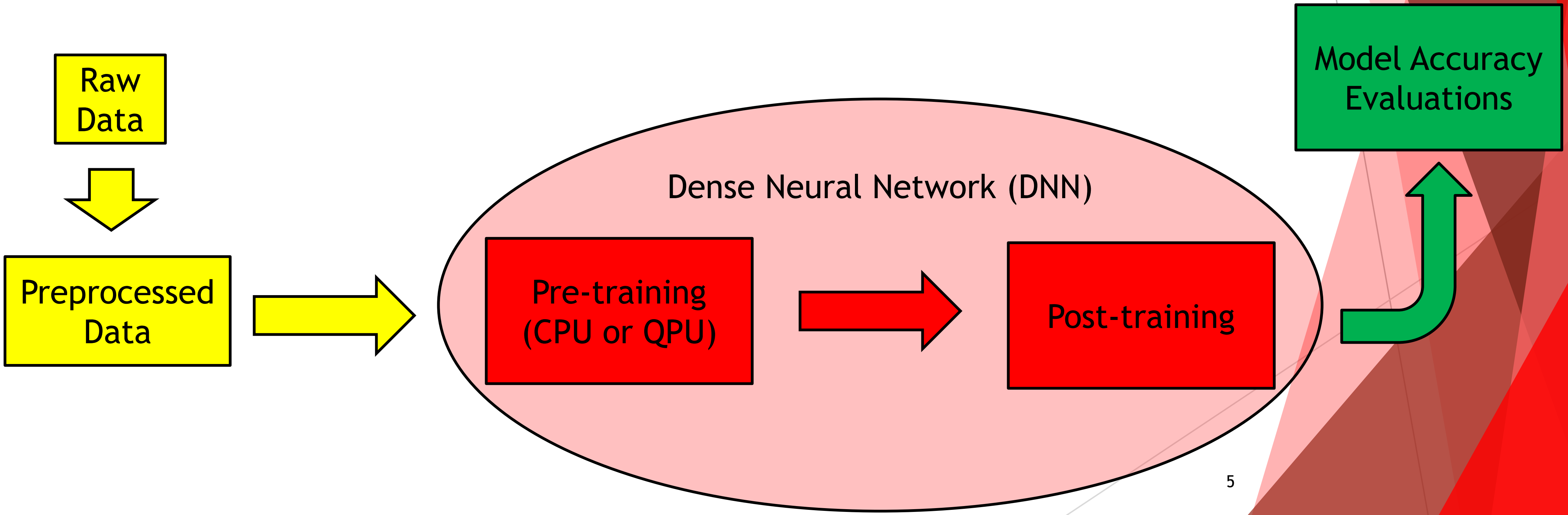

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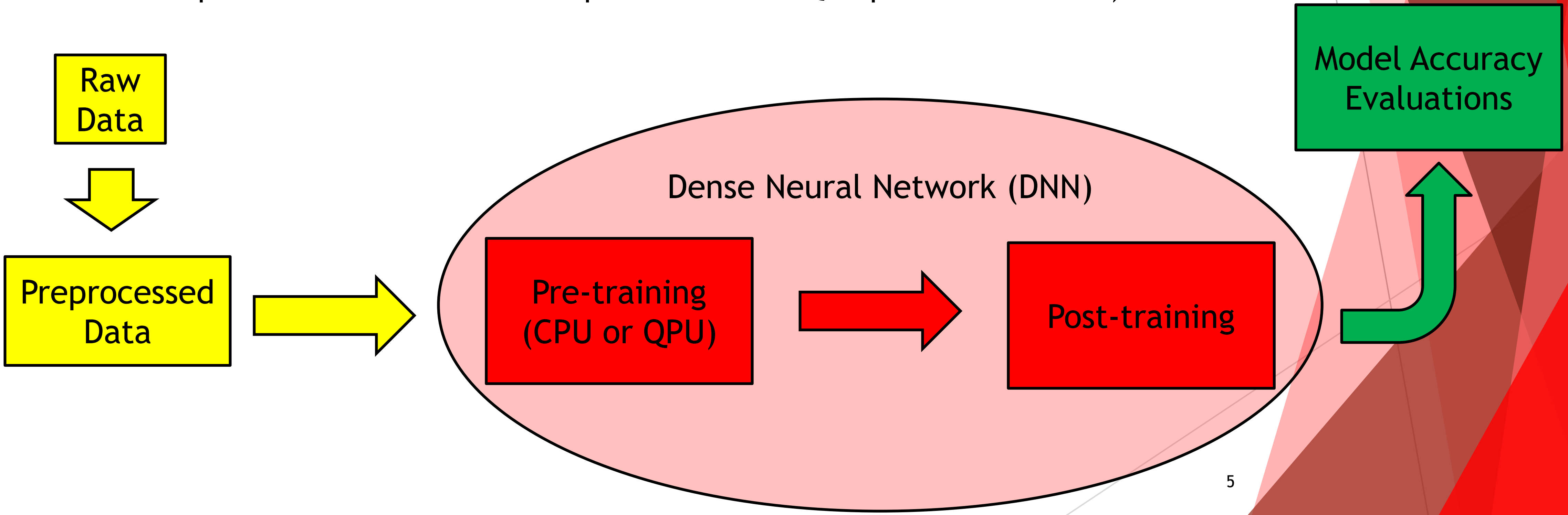
- This project's goal is to repeat their experiment (build the pipeline and evaluate performance between CPU-pre-trained vs. QPU pre-trained DNNs)



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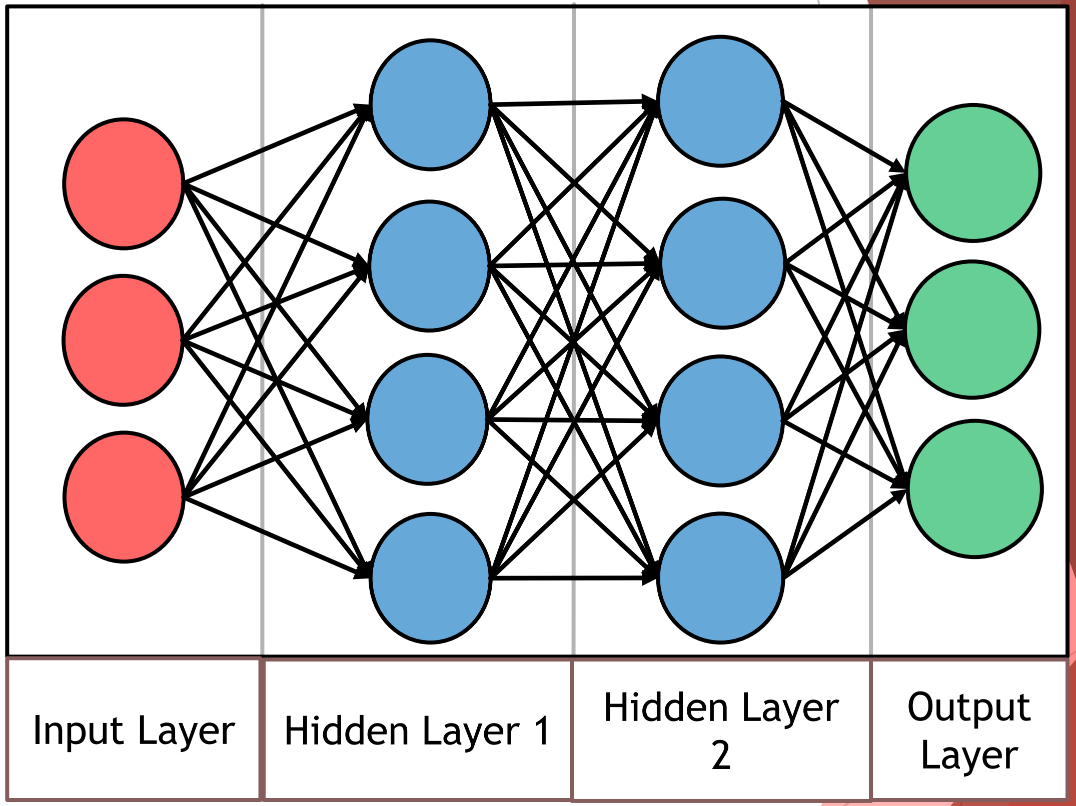

Graph model of a Dense Neural Network

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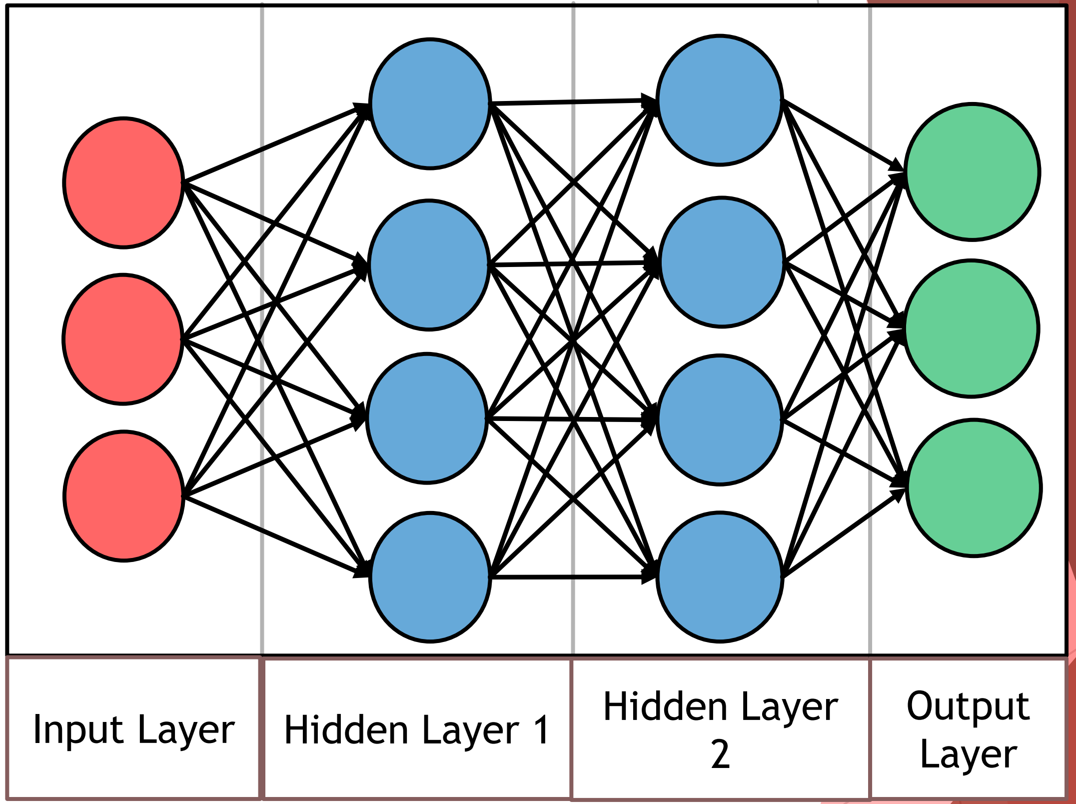

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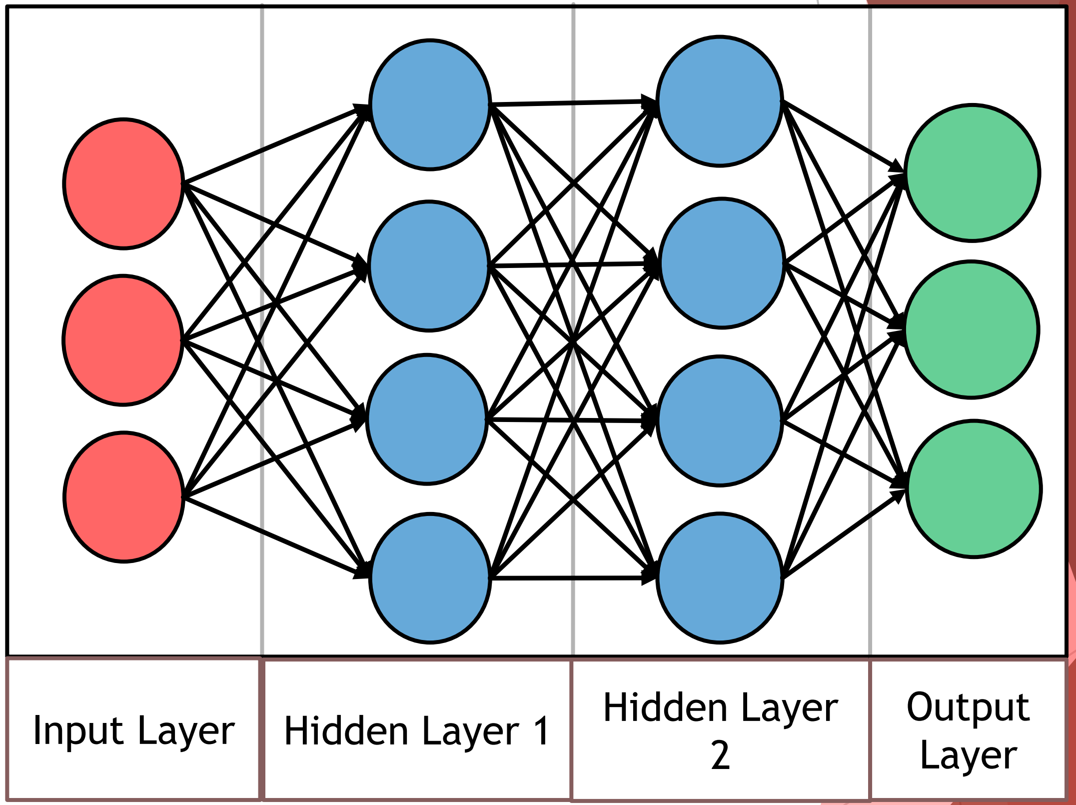

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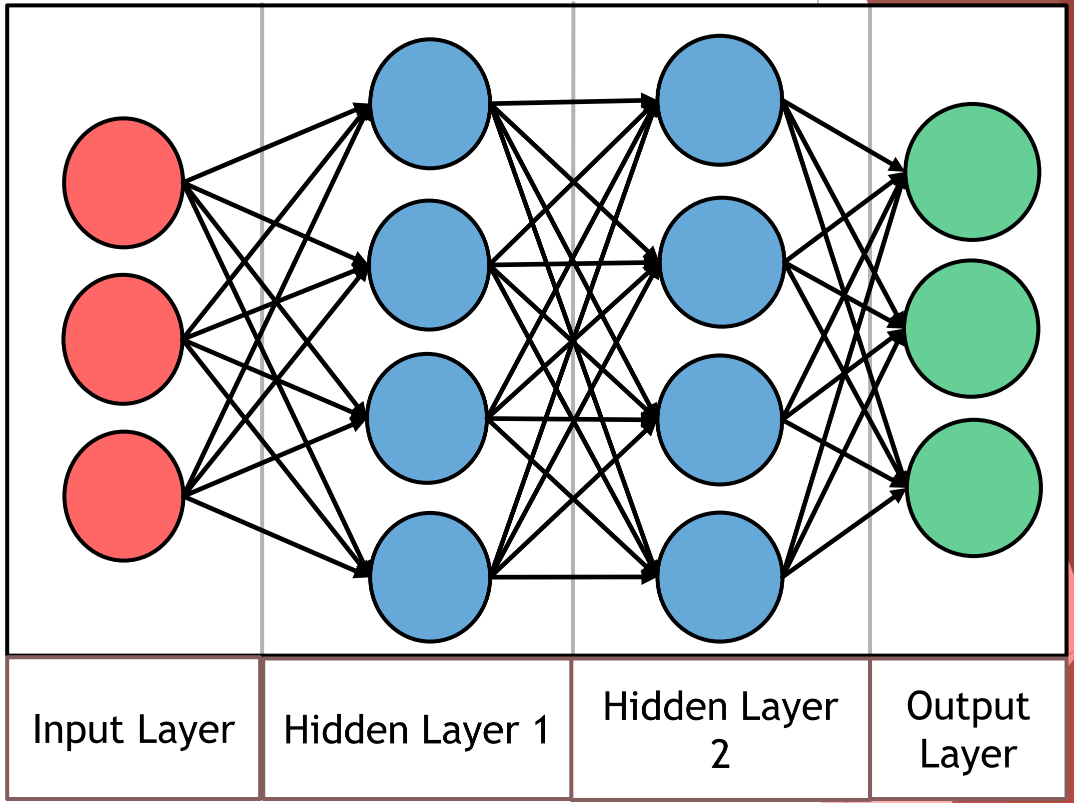

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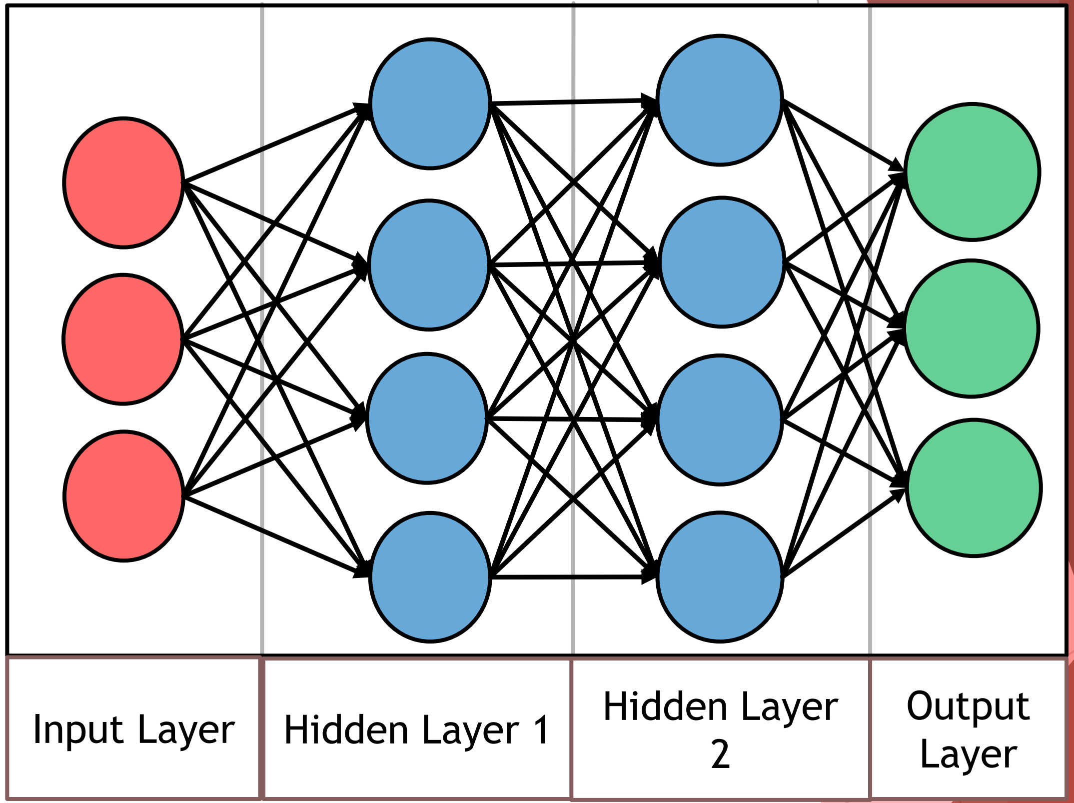
- Discovered that training a DNN using unsupervised learning technique can subsequently help the DNN train faster with supervised learning technique



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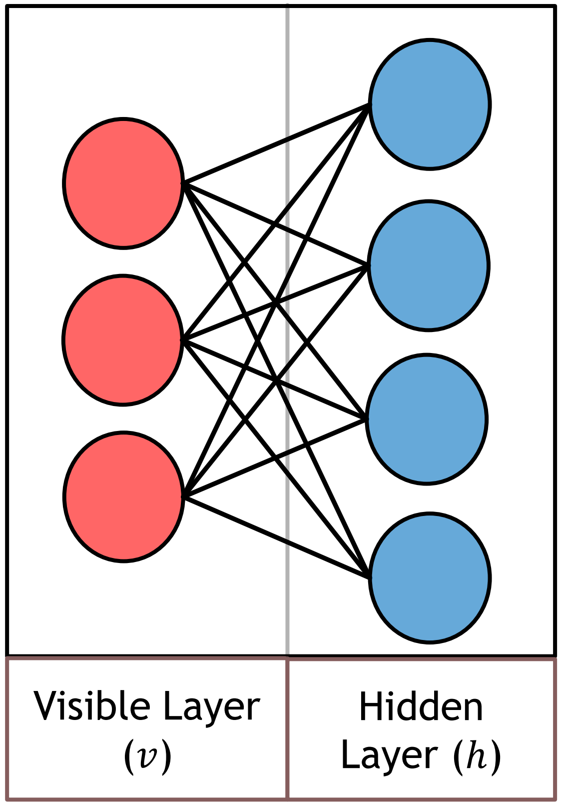

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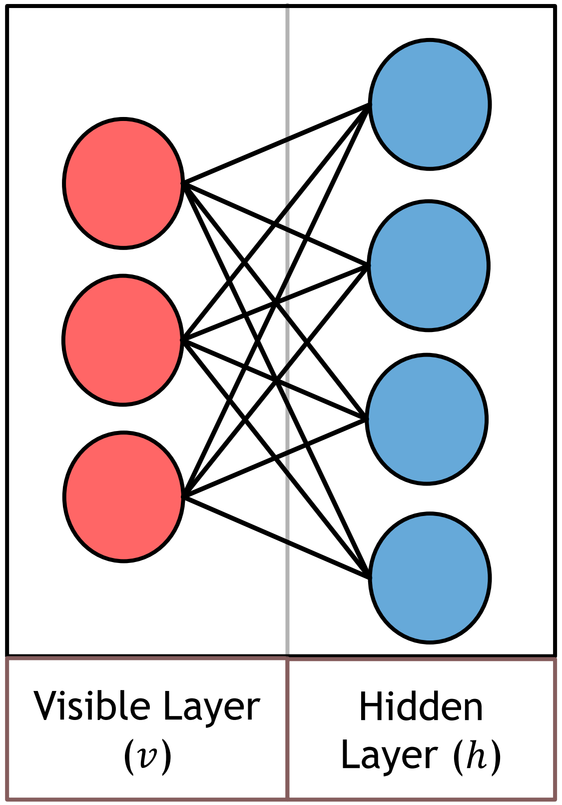

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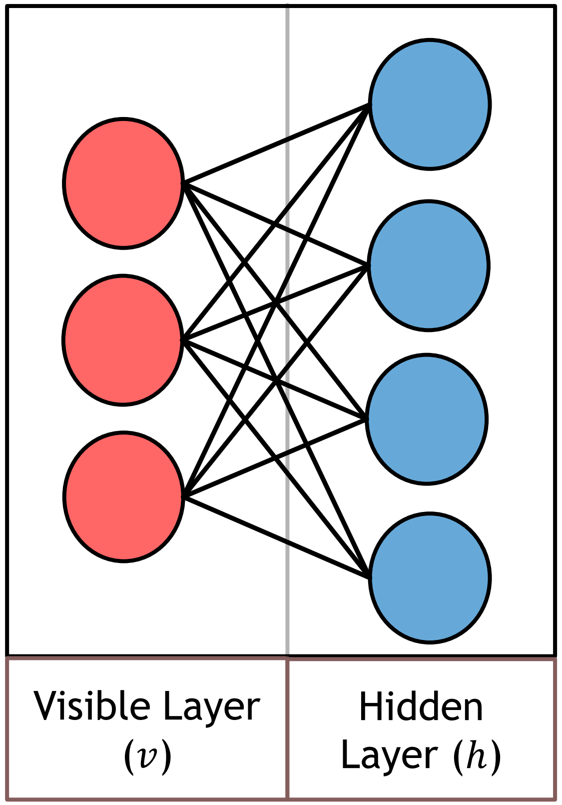

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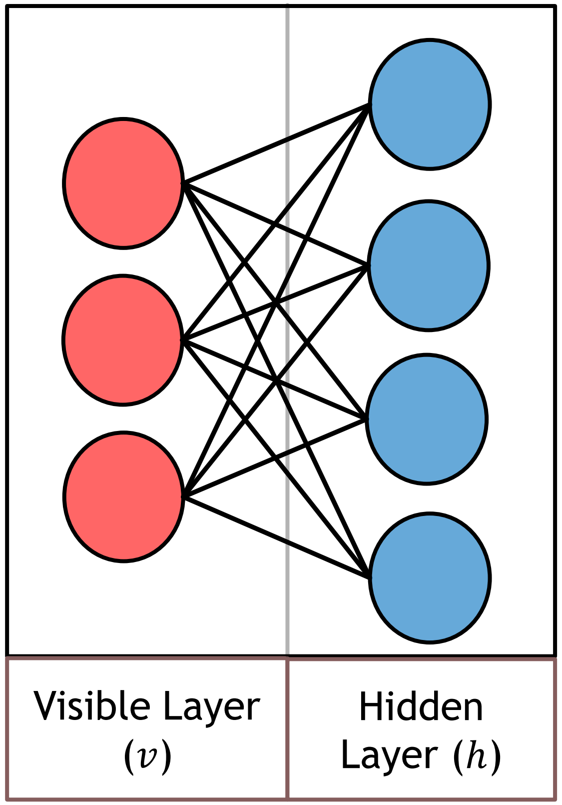

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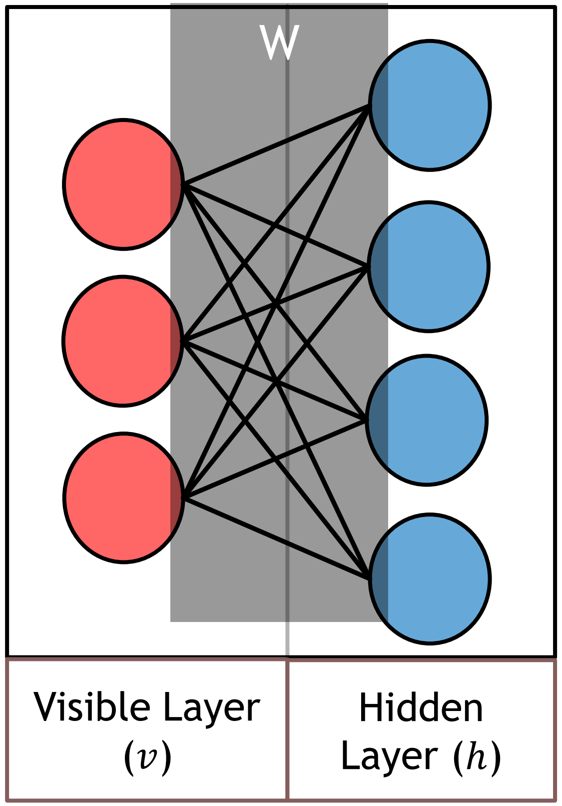

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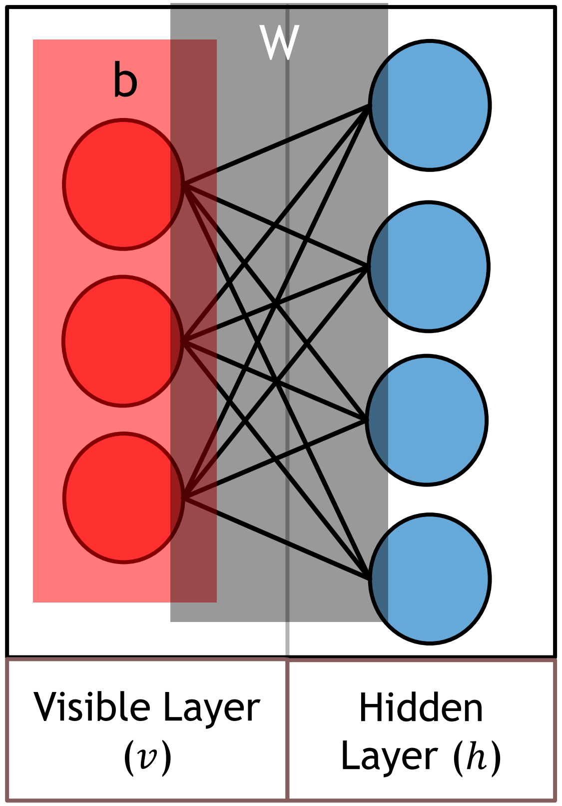

Graph model of an RBM

Restricted Boltzmann Machines (RBMs)

- Type of unsupervised learning model that models the presence of data as a Boltzmann distribution
  - When trained, it learns the probability distribution of given training data
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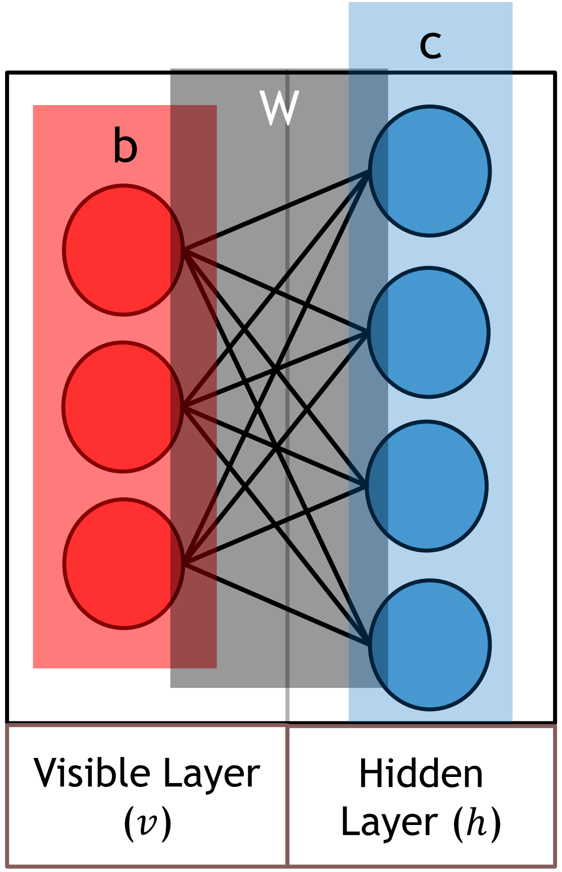

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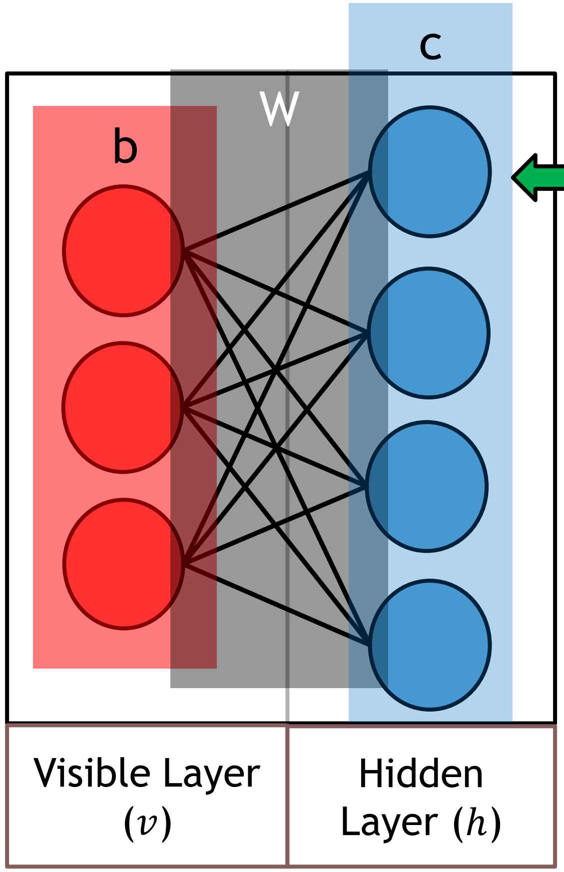

$P(h_0 = 1|v)$
$= \text{sigm}(W_{00}v_0 + W_{10}v_1 + W_{20}v_2 + c_0)$

Graph model of an RBM

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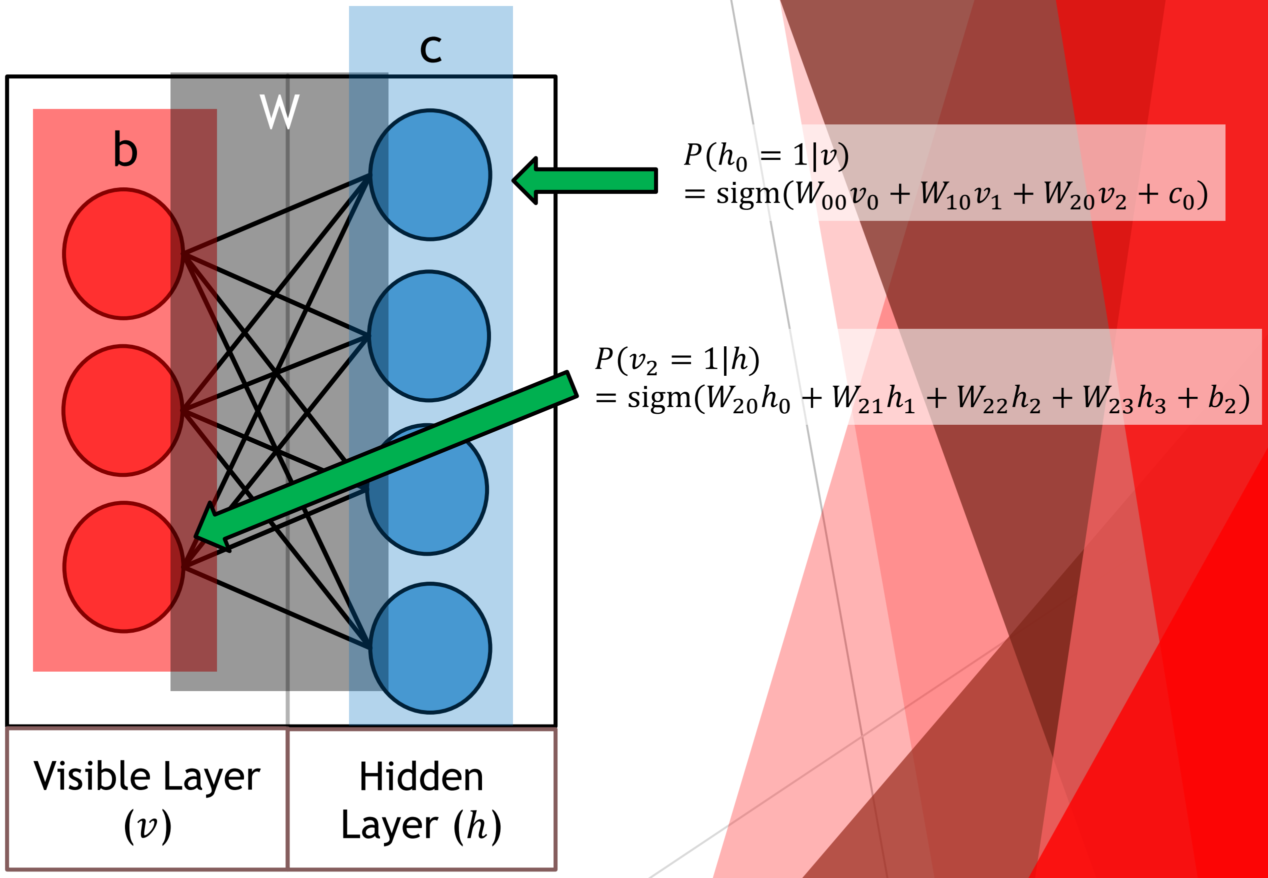
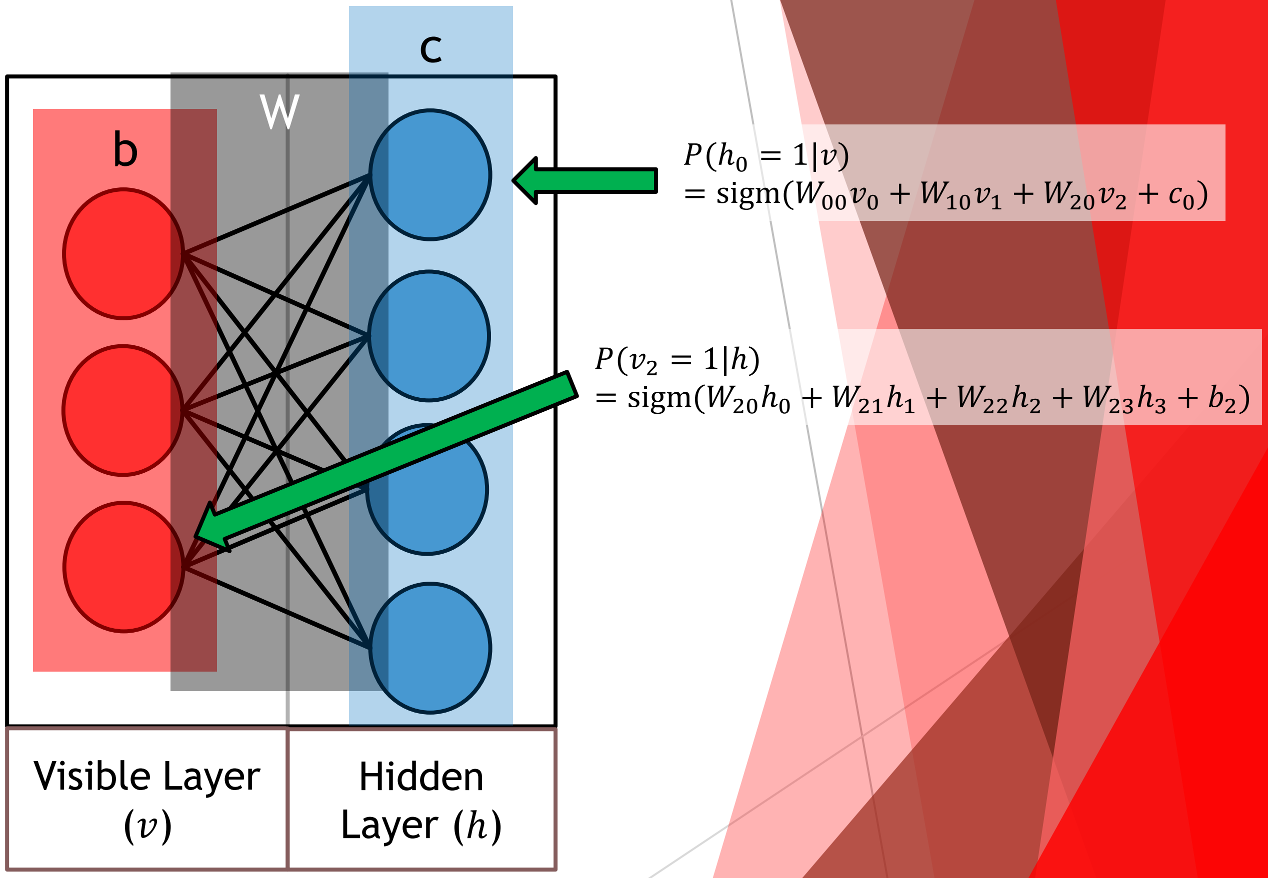


Graph model of an RBM

Restricted Boltzmann Machines (RBMs)

- Type of unsupervised learning model that models the presence of data as a Boltzmann distribution
  - When trained, it learns the probability distribution of given training data
  - Model parameters are weights (W), visible layer biases (b), and hidden layer biases (c)
- Variety of applications



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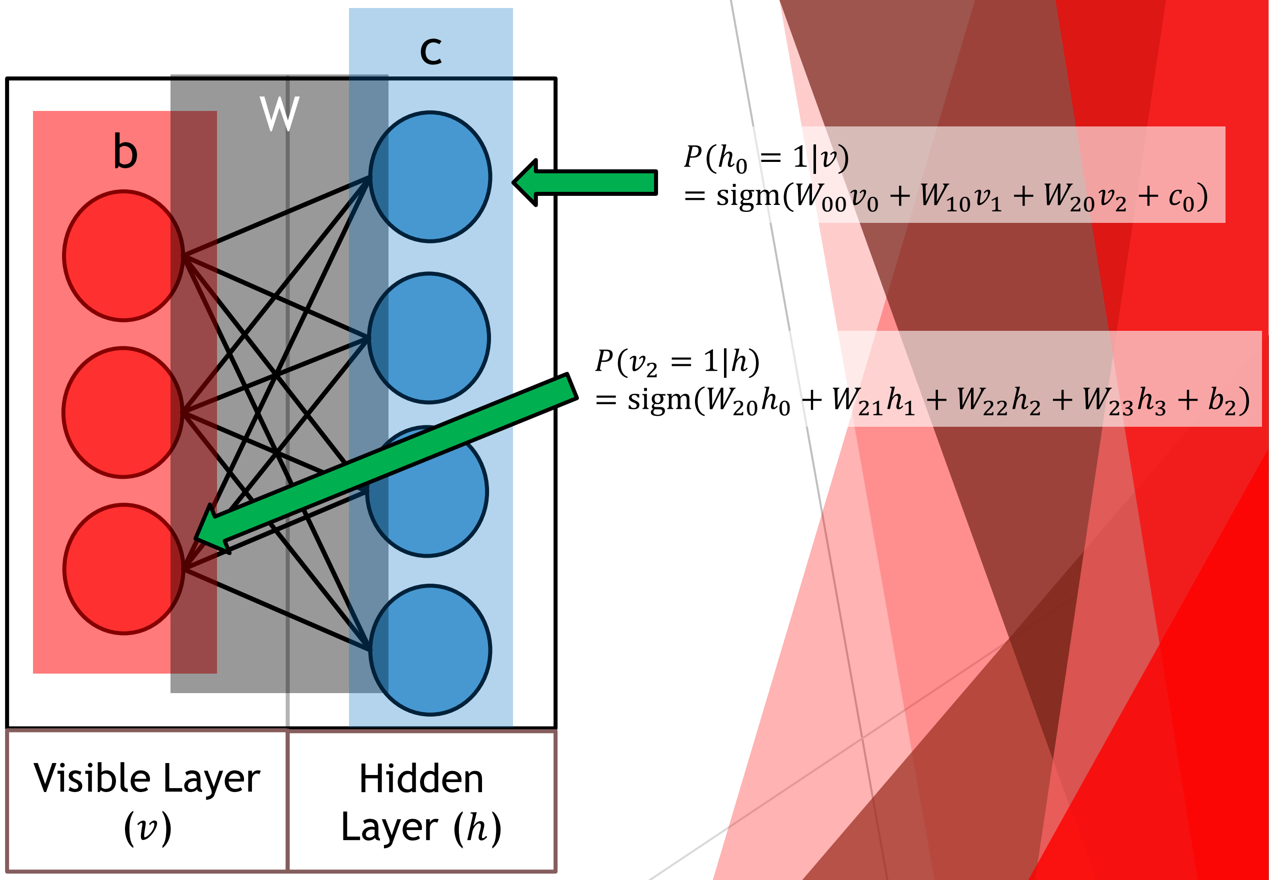
  - Fix the visible layer, and probabilistically "generate" hidden layer values – used for classification



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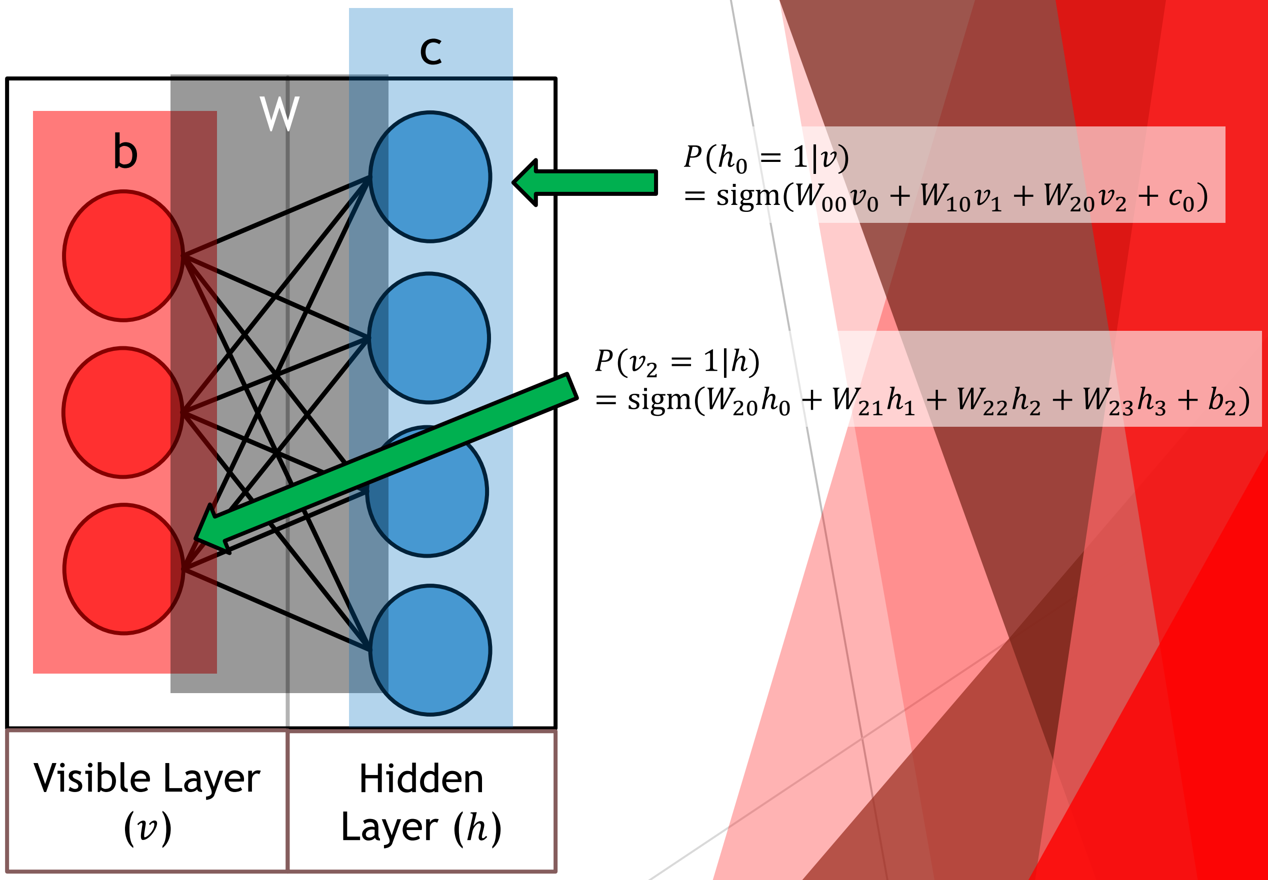
  - Fix the hidden layer, and probabilistically "generate" visible layer values – used for producing generative examples of a certain class



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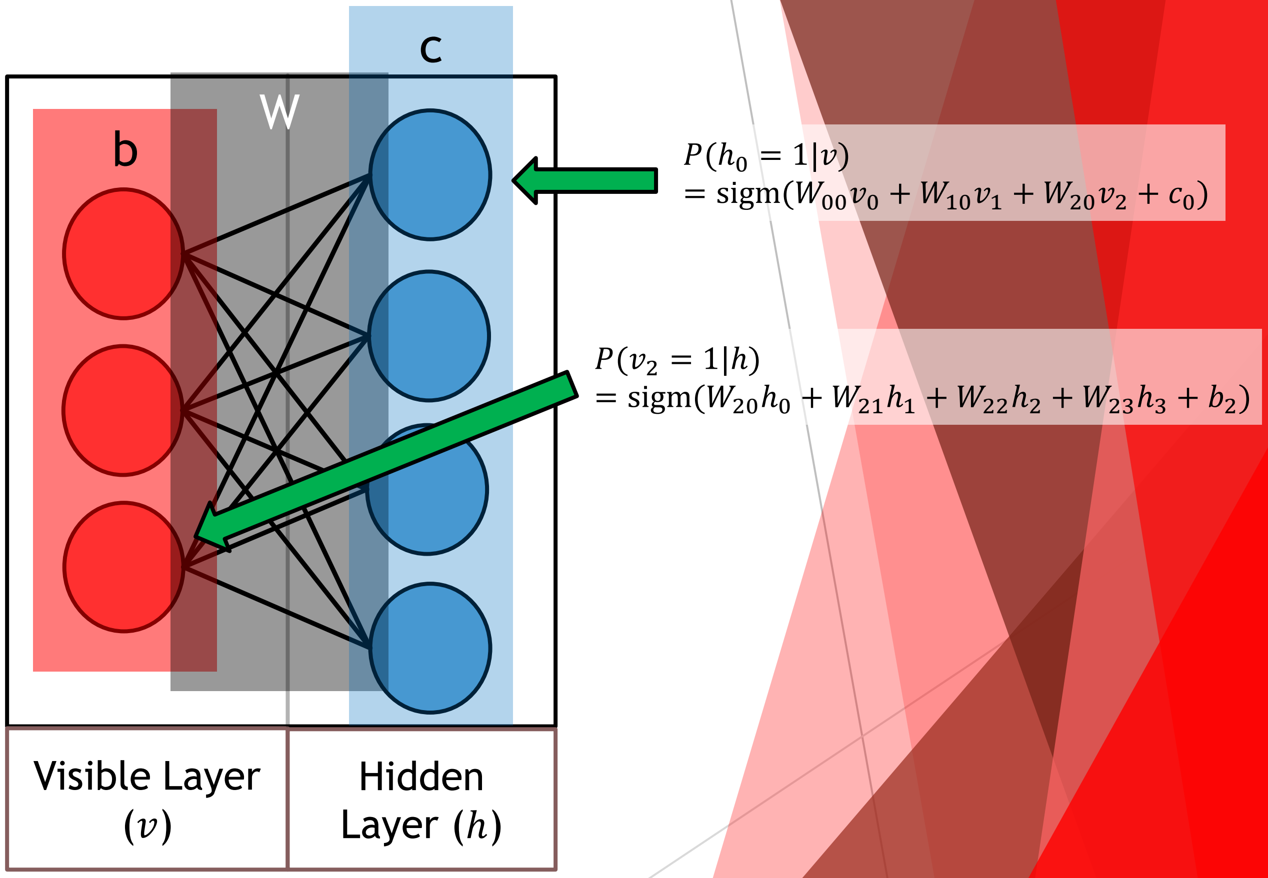
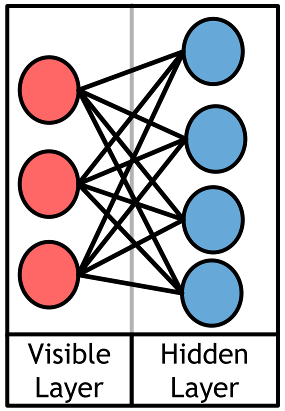
  - Fix the visible layer, and probabilistically “generate” hidden layer values – used for classification
  - Fix the hidden layer, and probabilistically “generate” visible layer values – used for producing generative examples of a certain class
  - Fix visible layer and generate hidden layer values, then fix generated hidden layer values to generate visible layer values - generating reconstructions of input data



Graph model of an RBM

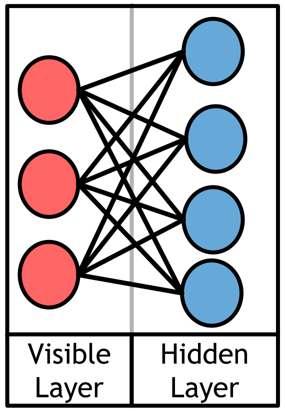
Deep Belief Networks



Graphical model of an RBM

Deep Belief Networks

- When multiple RBMs are stacked in a set of layers, they form a Deep Belief Network (DBN), which shares the same graph structure as a DNN



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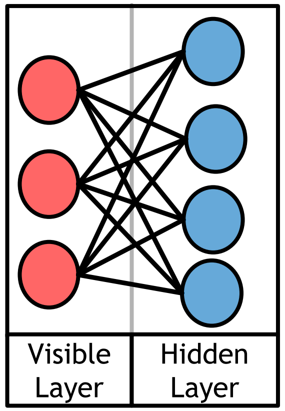

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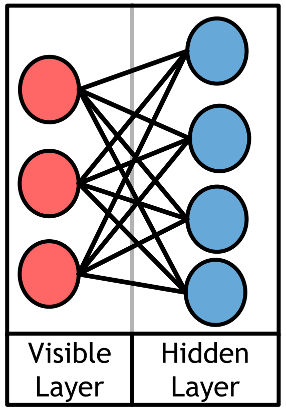

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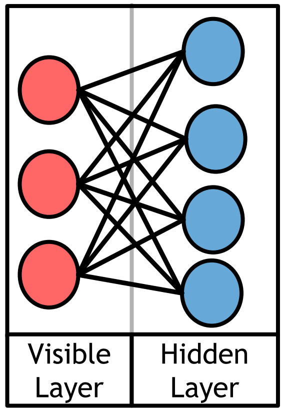

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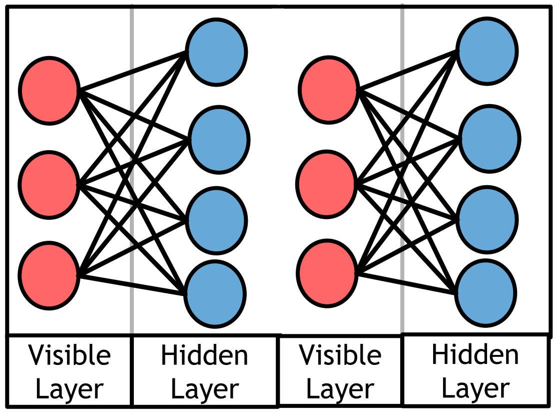

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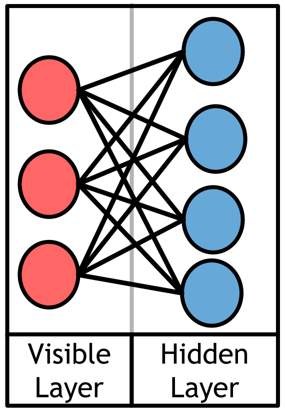

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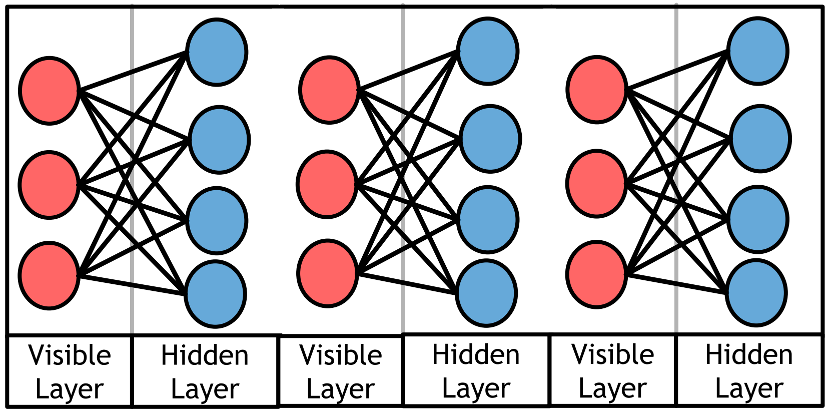

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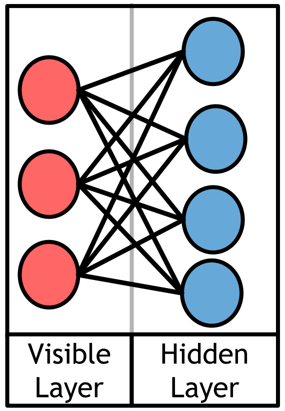
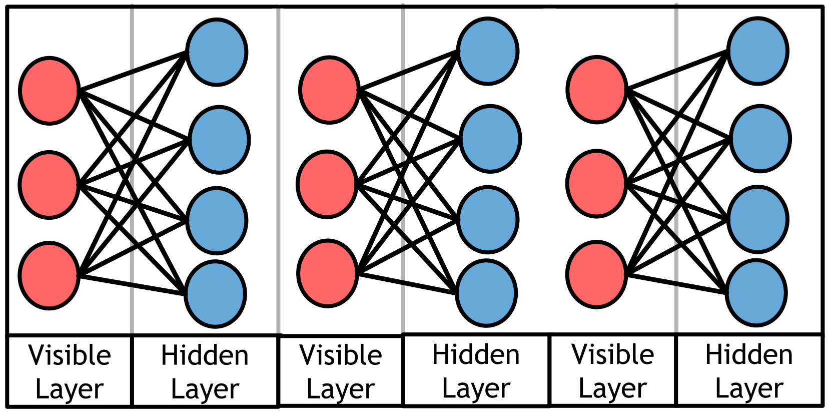


Graphical model of an RBM



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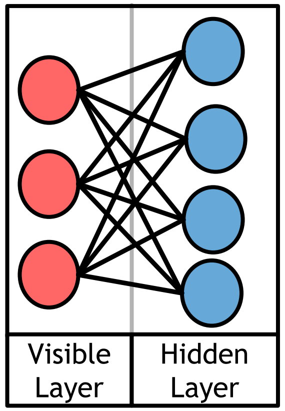
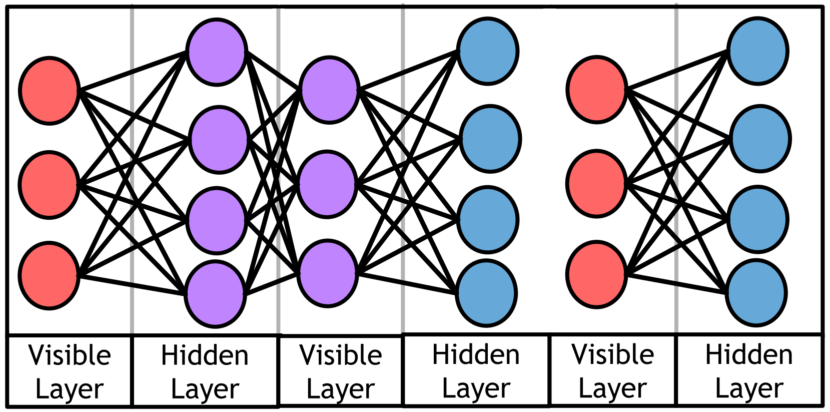


Graphical model of an RBM



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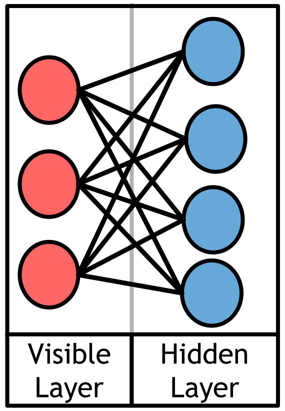

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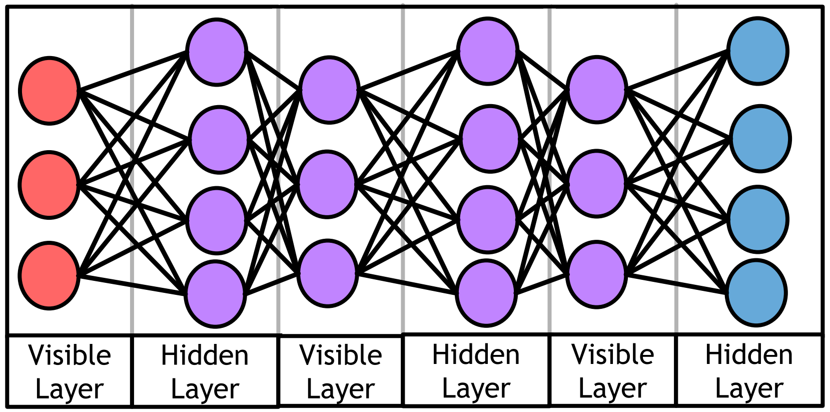

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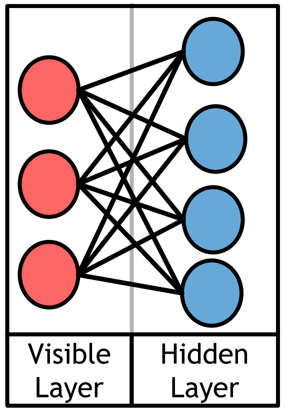
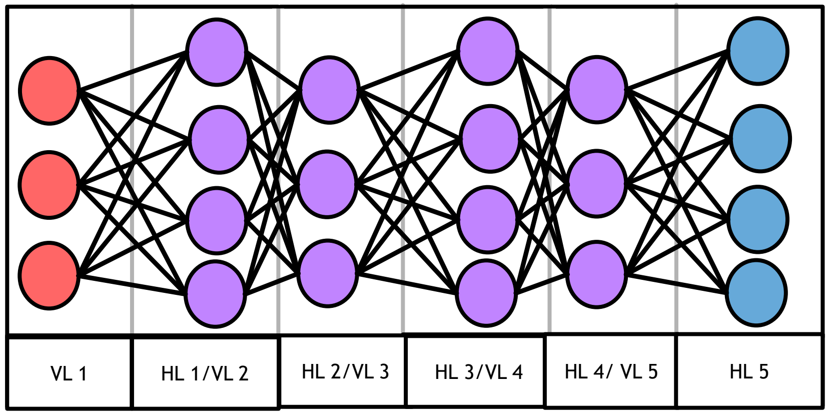


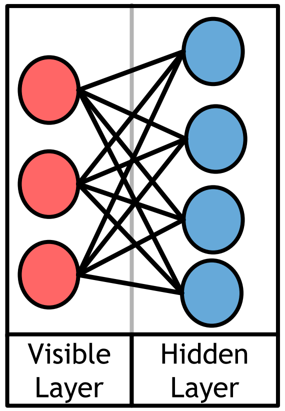
Graphical model of an RBM



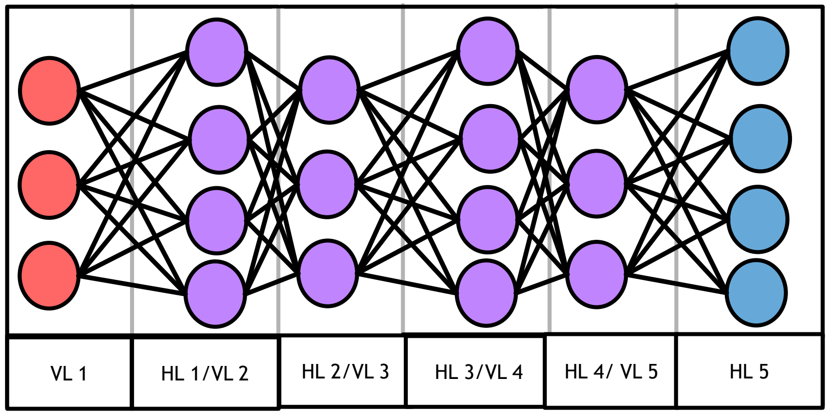
Graphical model of a DBN

Deep Belief Networks

- When multiple RBMs are stacked in a set of layers, they form a Deep Belief Network (DBN), which shares the same graph structure as a DNN
- Observed that DNNs trained with stochastic gradient descent with backpropagation with initial weights and biases determined from equivalently-structured pre-trained DBNs perform significantly better than non-pre-trained DNNs (Erhan et al. 2010)



Graphical model of an RBM



Graphical model of a DBN

Training a Deep Belief Network

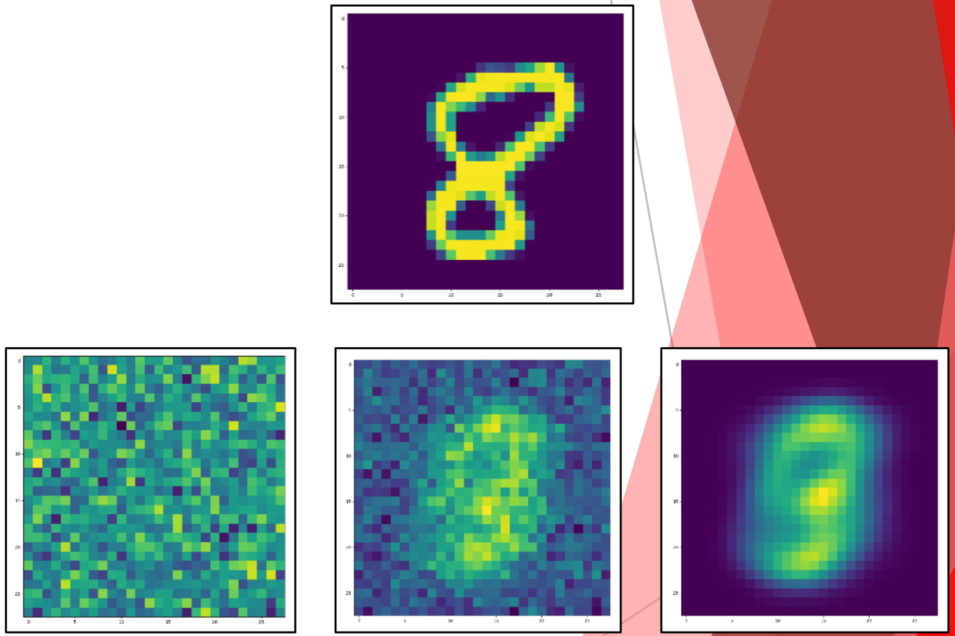
RBM weight update formulas:

CPU (CD):

$$w_{ij}^{(t+1)} = \alpha w_{ij}^{(t)} + \epsilon[\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{recon}]$$

QPU:

$$w_{ij}^{(t+1)} = \alpha w_{ij}^{(t)} + \epsilon[\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{model}]$$



(Top) Original MNIST training image (Bottom, Left to Right) Reconstructions of the original image above with DBN models trained with 0, 1, and 10 iterations, respectively

Training a Deep Belief Network

- DBNs are trained sequentially, training every pair of adjacent layers as an RBM, from the input layer + the first hidden layer to the 2nd-to-last hidden layer + the last hidden layer

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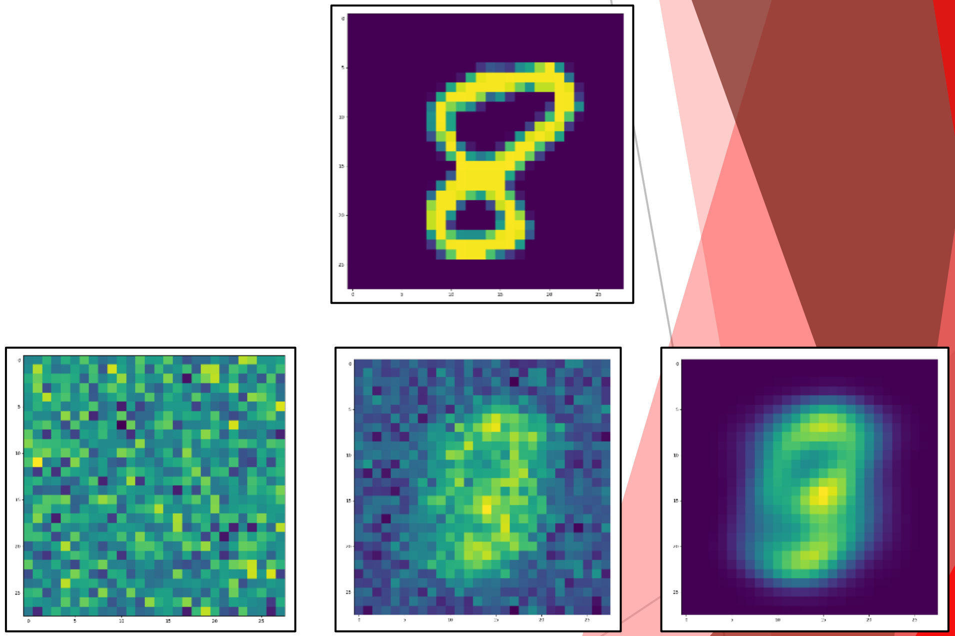

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Training a Deep Belief Network

- DBNs are trained sequentially, training every pair of adjacent layers as an RBM, from the input layer + the first hidden layer to the 2nd-to-last hidden layer + the last hidden layer
  - Known as "generative training"

RBM weight update formulas:

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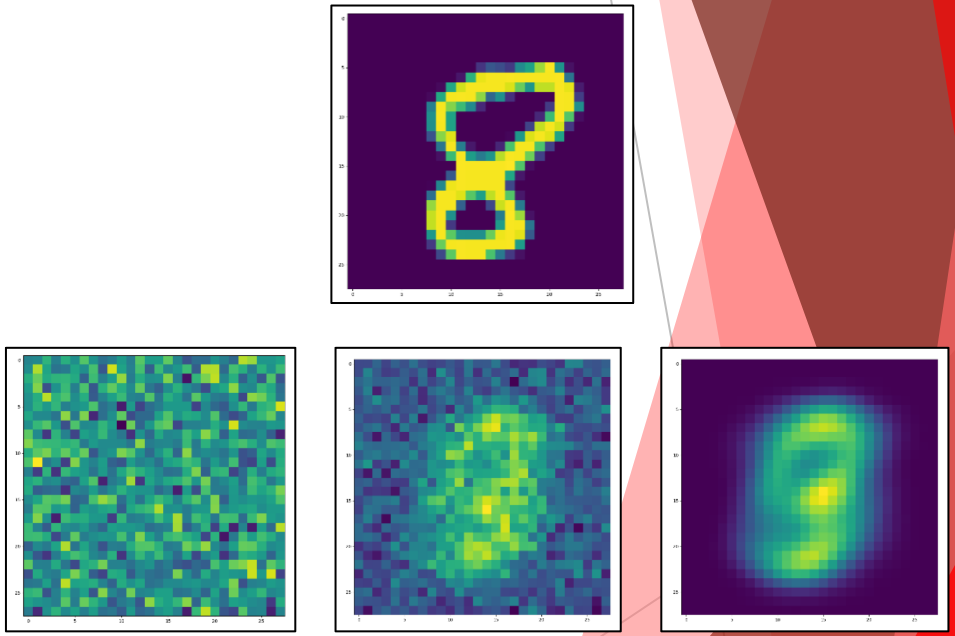

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- RBM training algorithm: Contrastive Divergence (CD); for each iteration of CD:

RBM weight update formulas:

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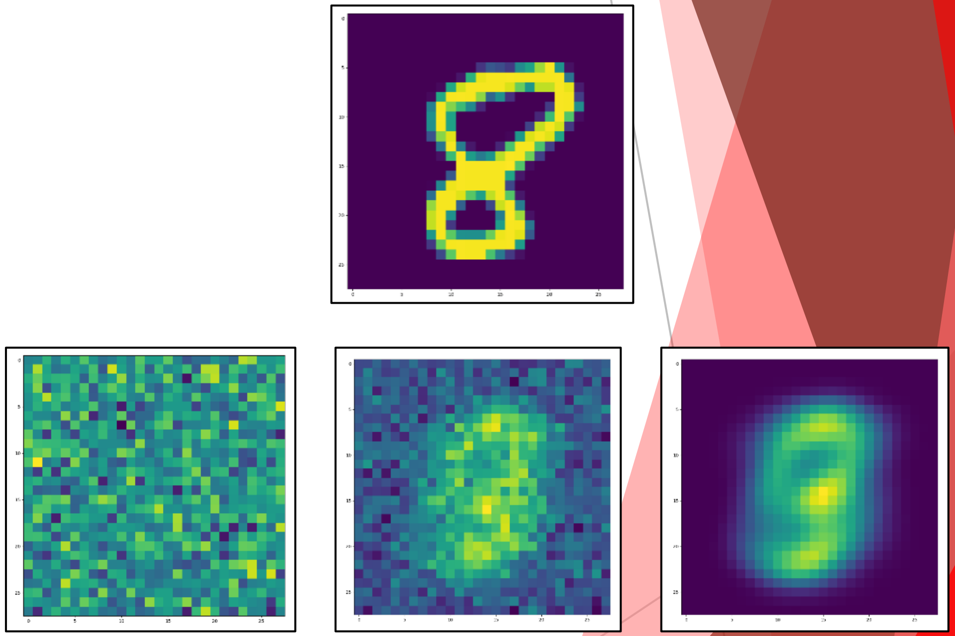

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  - Create a reconstruction of the original data using the RBM

RBM weight update formulas:

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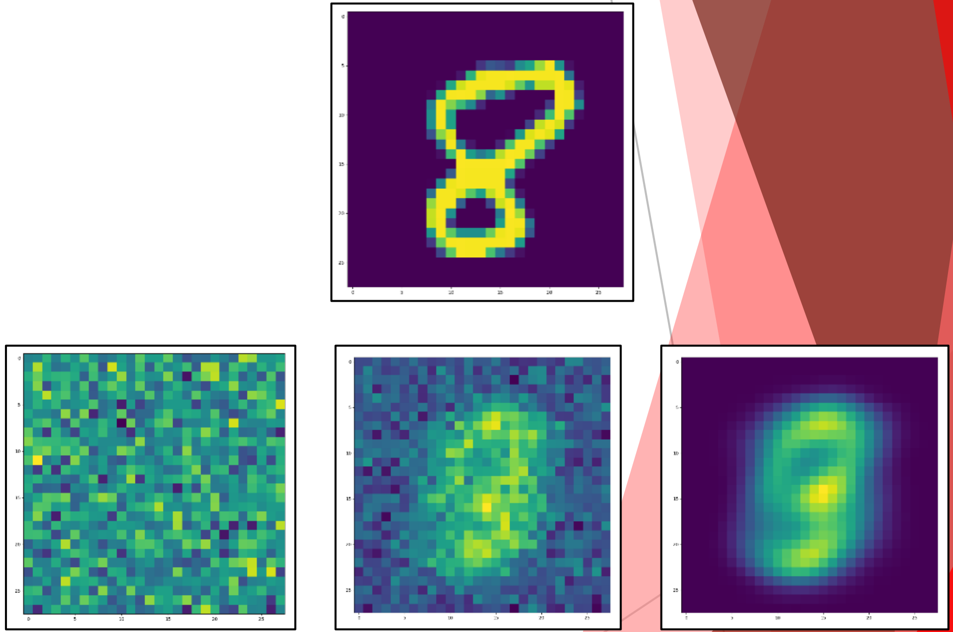

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- RBM training algorithm: Contrastive Divergence (CD); for each iteration of CD:
  - Create a reconstruction of the original data using the RBM
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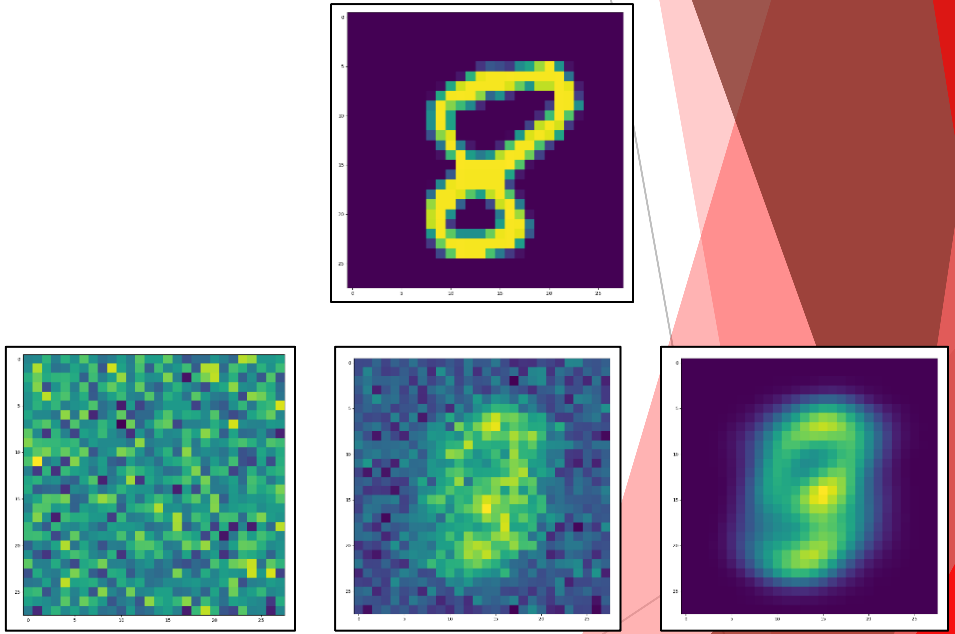

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- RBM training algorithm: Contrastive Divergence (CD); for each iteration of CD:
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  - Apply slight corrections the weights and biases of the RBM to make the RBM more accurate

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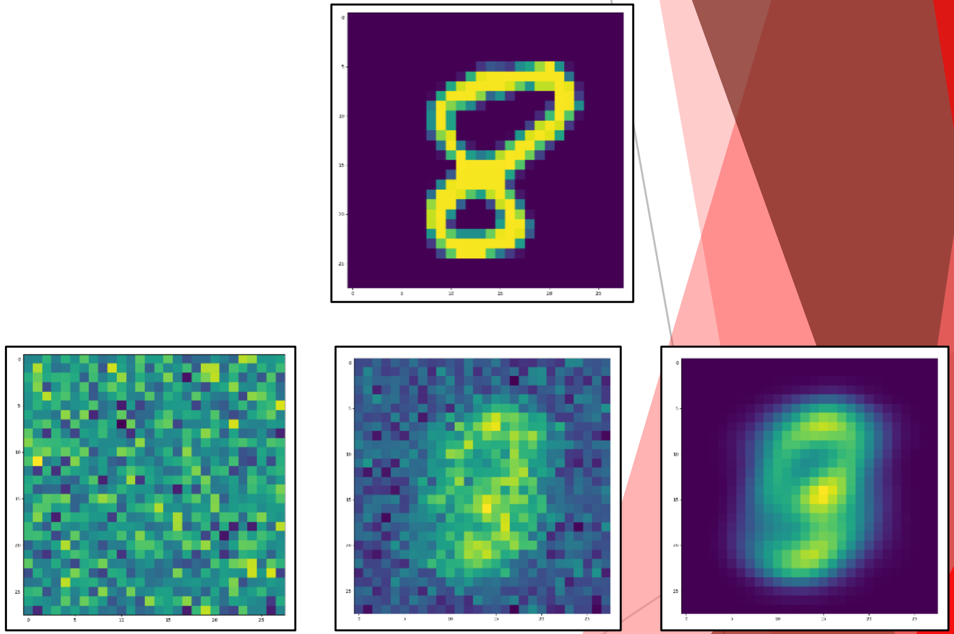

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- Problem with CD method: Slow convergence for learning

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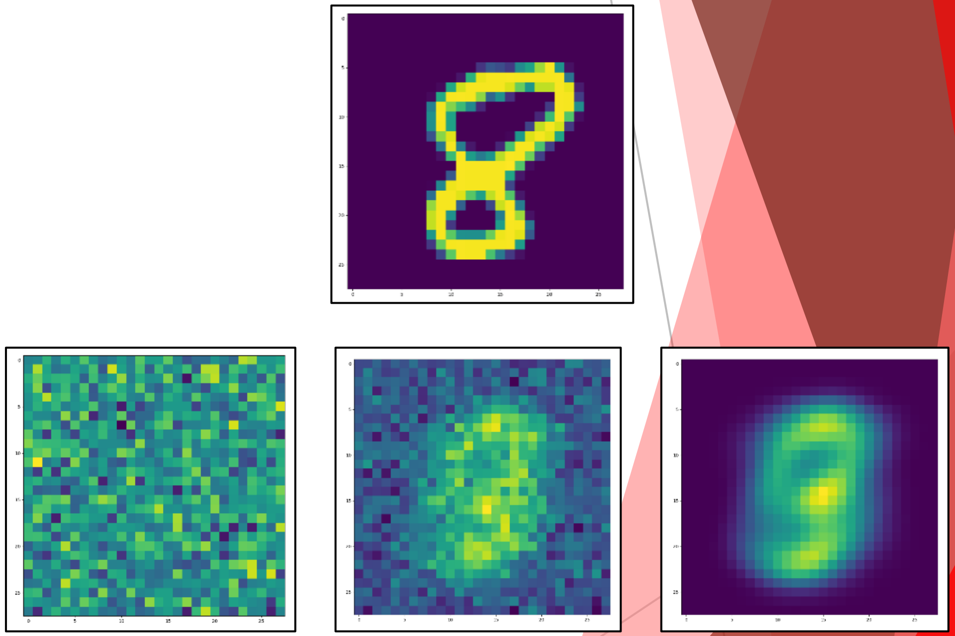

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  - takes many iterations to minimize loss (error) function

RBM weight update formulas:

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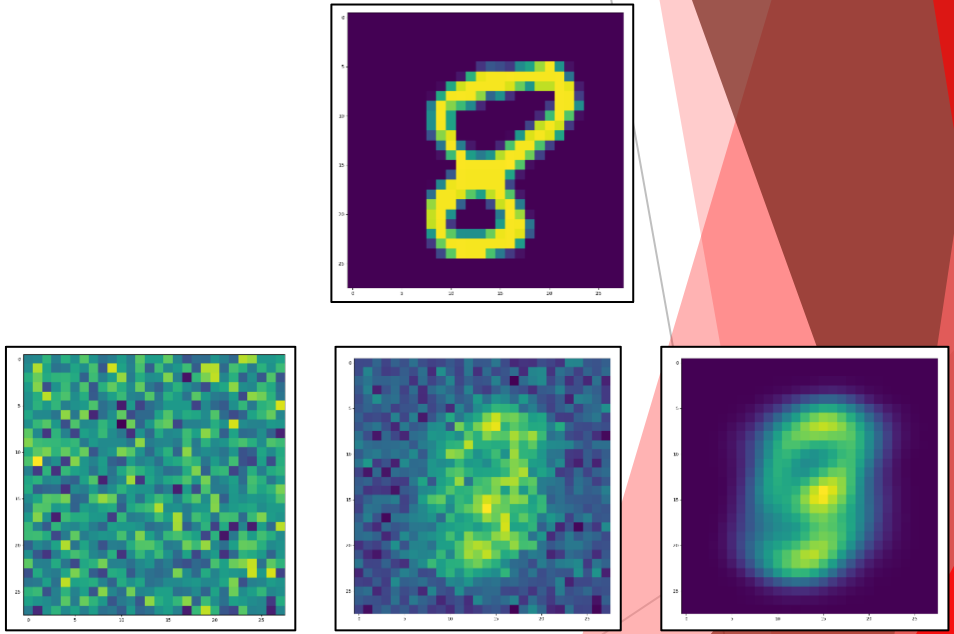

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- Problem with CD method: Slow convergence for learning
  - takes many iterations to minimize loss (error) function
- Possible solution: Training using a quantum computer

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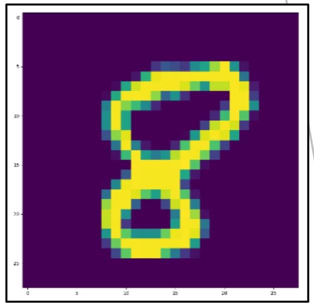

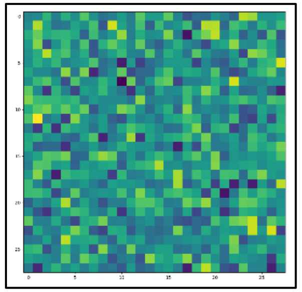

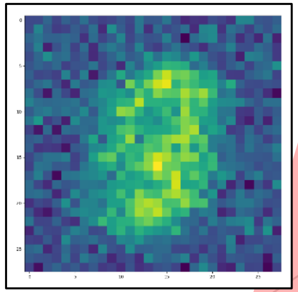

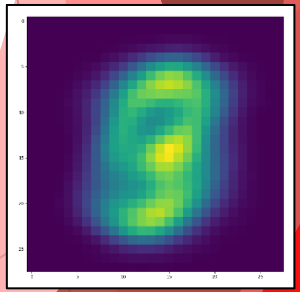

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- DBNs are trained sequentially, training every pair of adjacent layers as an RBM, from the input layer + the first hidden layer to the 2nd-to-last hidden layer + the last hidden layer
  - Known as “generative training”
- RBM training algorithm: Contrastive Divergence (CD); for each iteration of CD:
  - Create a reconstruction of the original data using the RBM
  - Evaluate how close the reconstruction matches the original data
  - Apply slight corrections the weights and biases of the RBM to make the RBM more accurate
- Problem with CD method: Slow convergence for learning
  - takes many iterations to minimize loss (error) function
- Possible solution: Training using a quantum computer
  - Model visible and hidden layer values for RBM can be efficiently sampled using a quantum annealer, so the model expectation values can be found and the gradient formula to update the model weights and biases

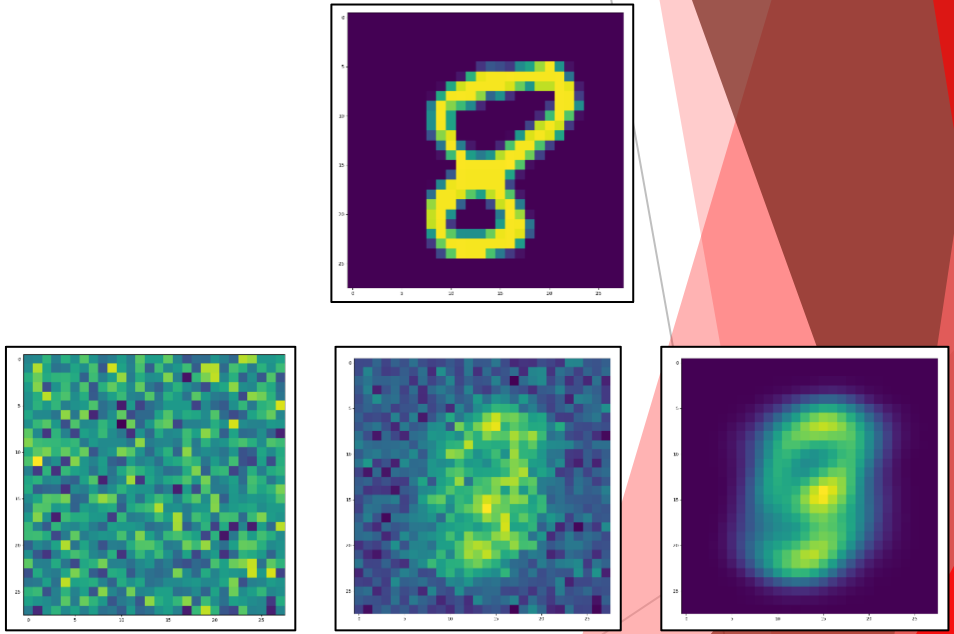
RBM weight update formulas:

CPU (CD):

$$w_{ij}^{(t+1)} = \alpha w_{ij}^{(t)} + \epsilon[\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{recon}]$$

QPU:

$$w_{ij}^{(t+1)} = \alpha w_{ij}^{(t)} + \epsilon[\langle v_i h_j \rangle_{data} - \langle v_i h_j \rangle_{model}]$$



(Top) Original MNIST training image (Bottom, Left to Right) Reconstructions of the original image above with DBN models trained with 0, 1, and 10 iterations, respectively

Previous Research (Revisited)

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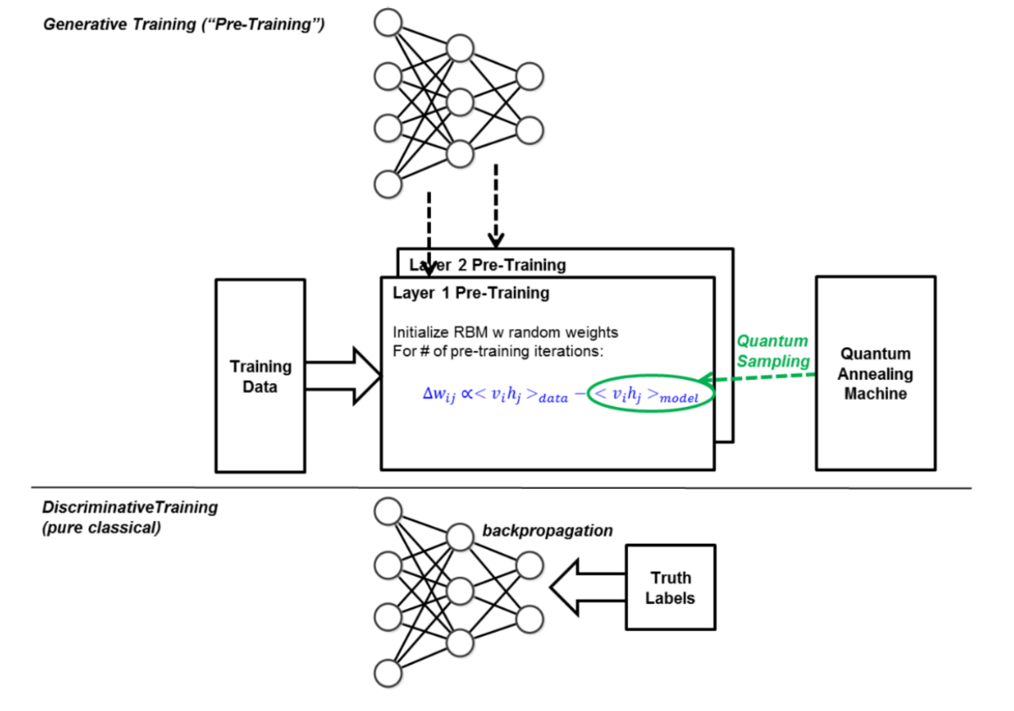

Figure 2 Overall training approach including generative and discriminative training

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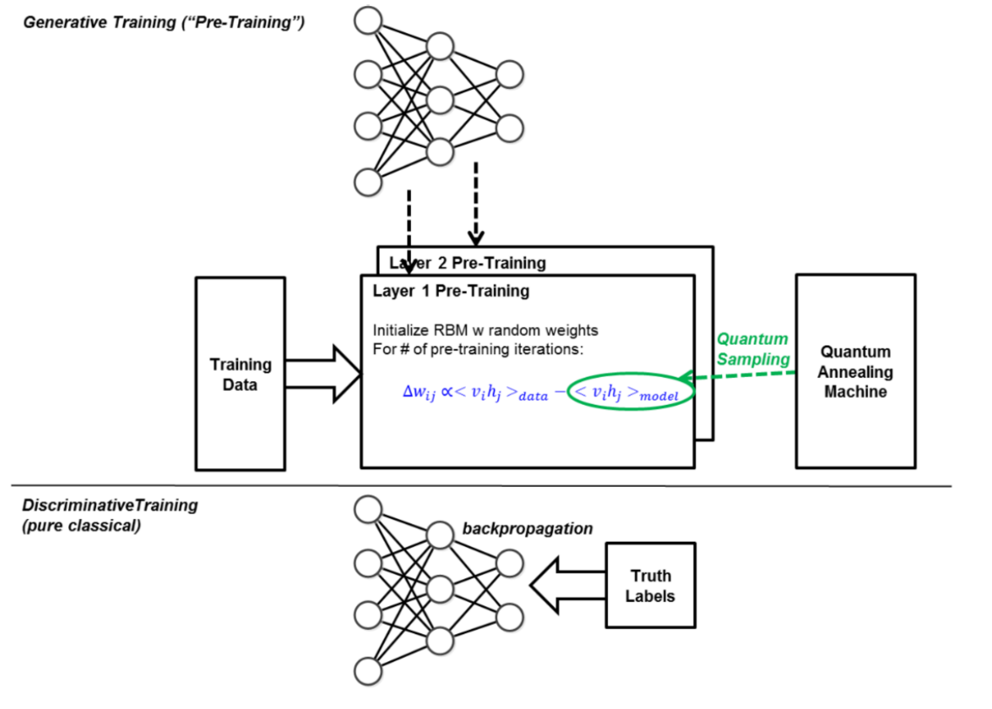

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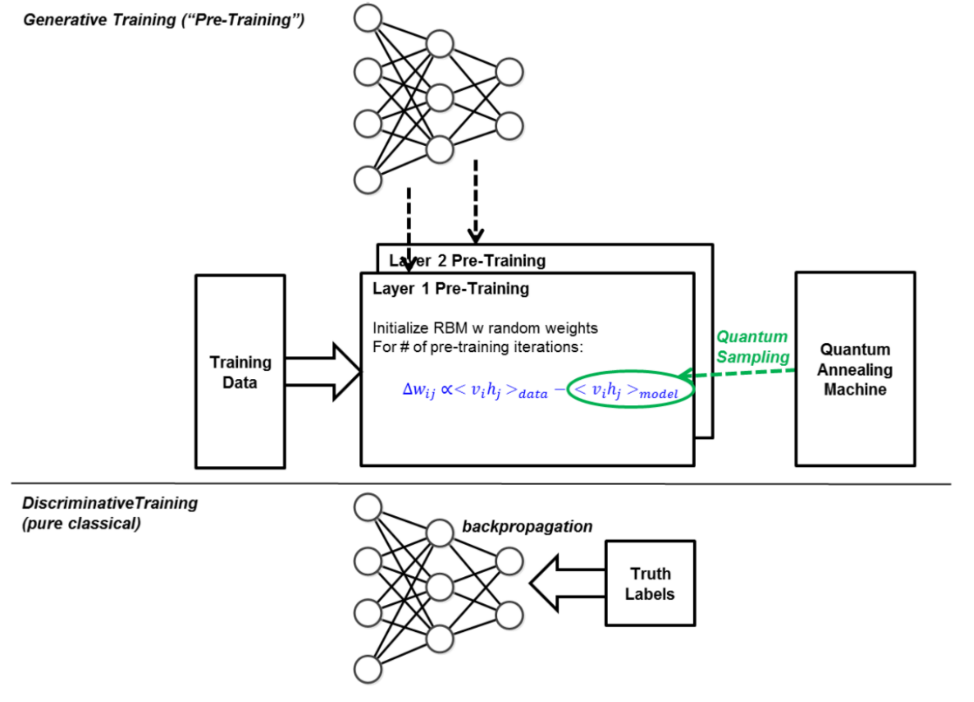

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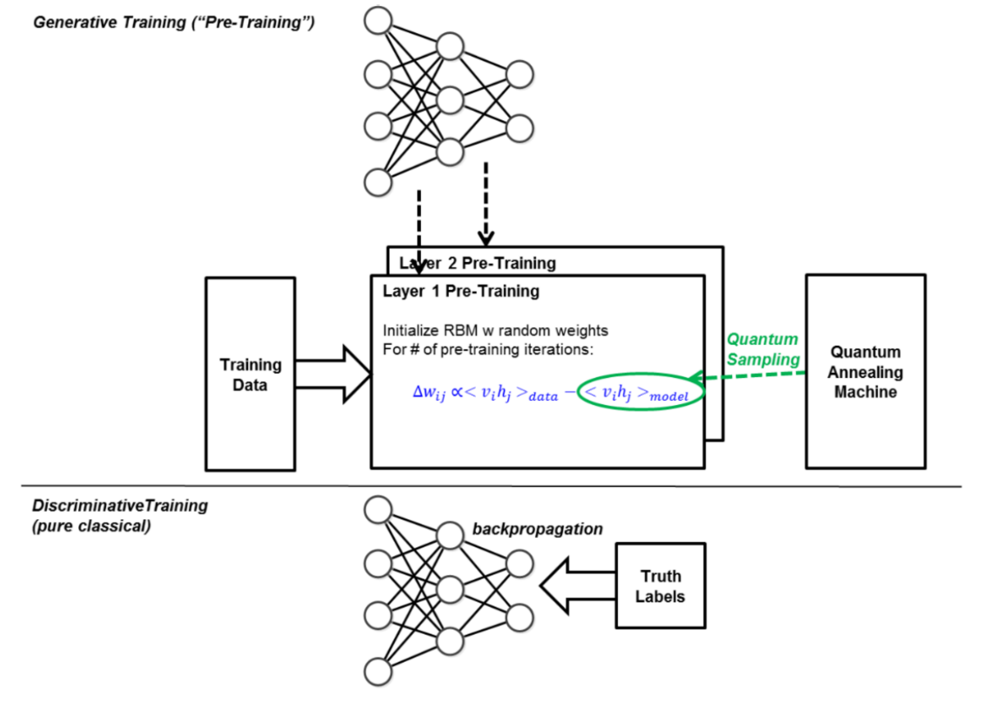

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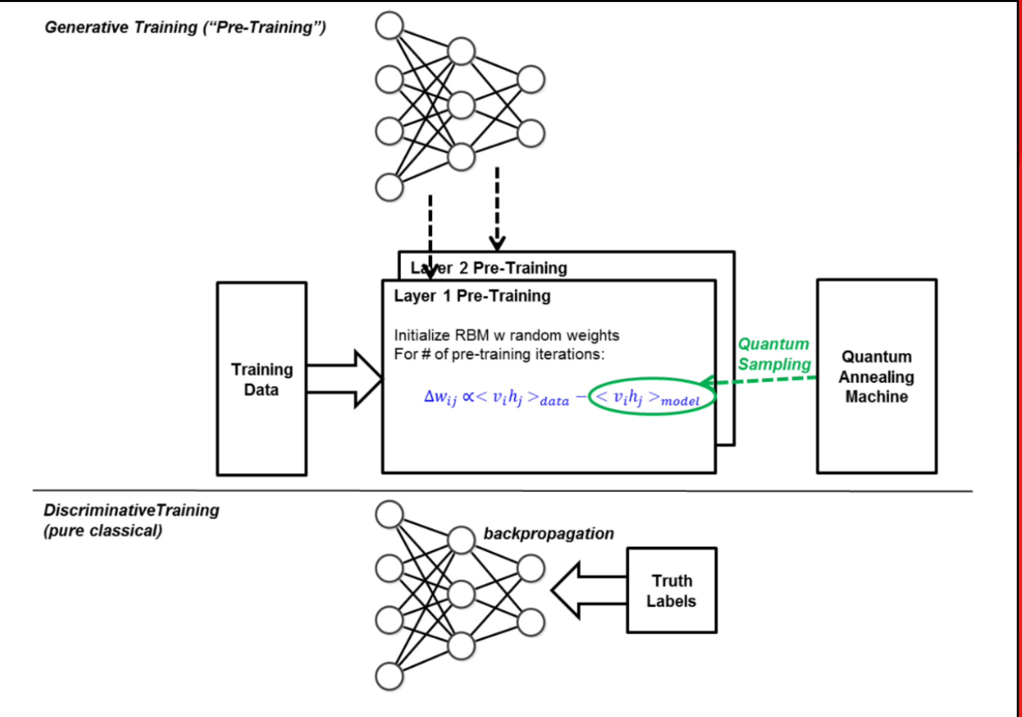

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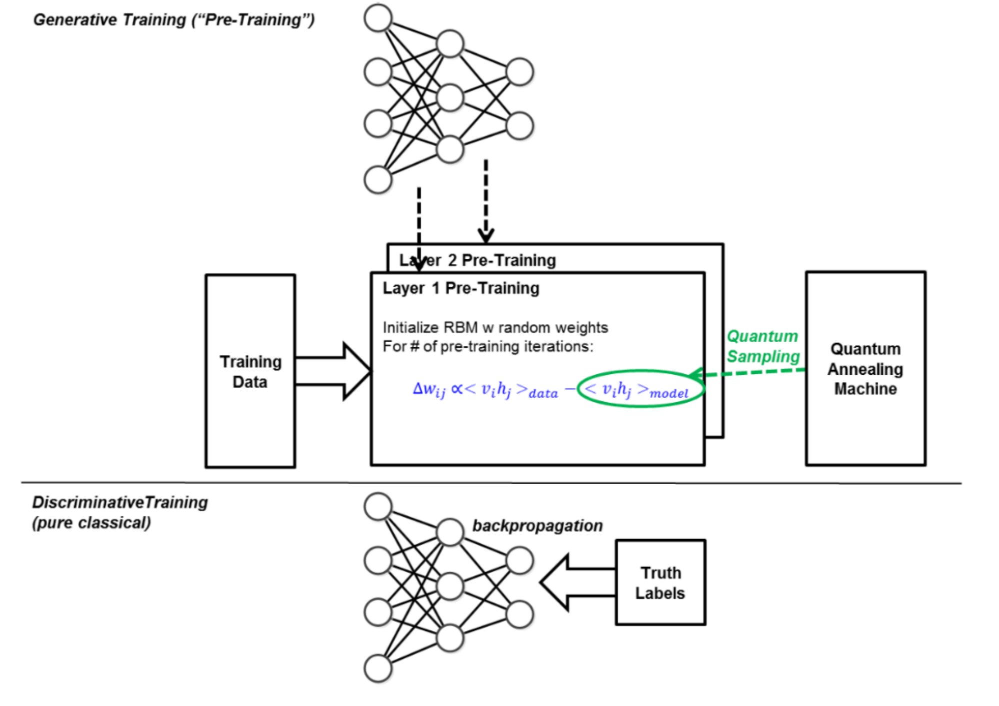
- This project's goal is to repeat their experiment



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Adachi & Henderson 2015

Implementation

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- Implementation divided into 3 major components

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  - Post-training learning curves (post-training accuracy vs. number of backpropagation iterations)

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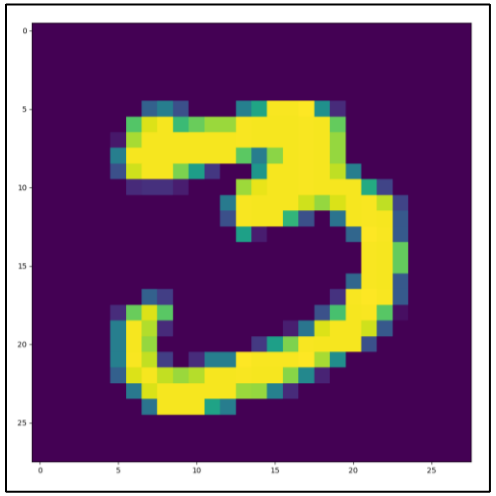
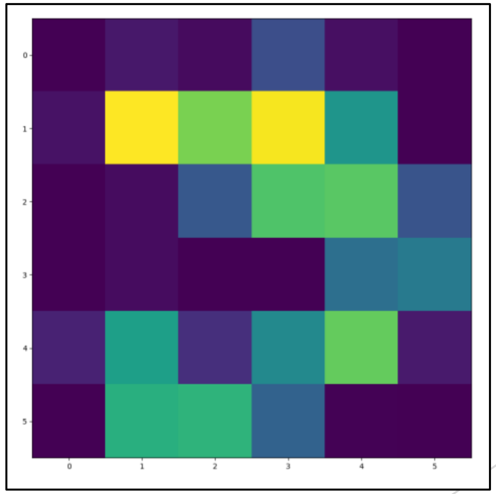
    - Main results to compare with Adachi & Henderson 2015 paper

Data Pre-processing Implementation Details



Example MNIST Image (Original)



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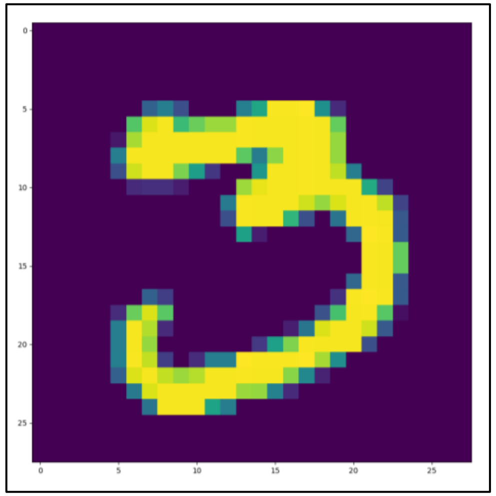

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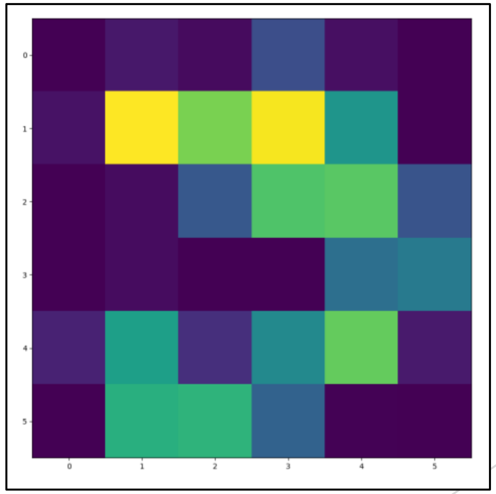

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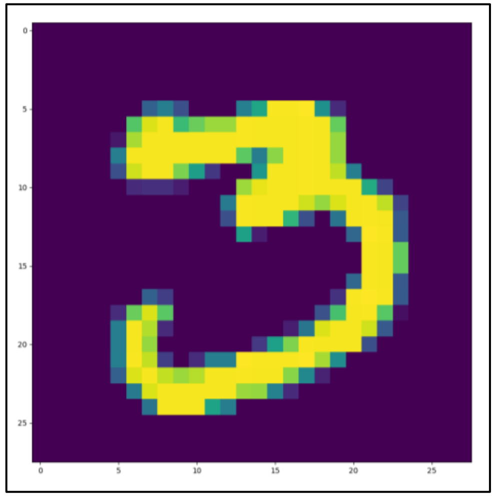

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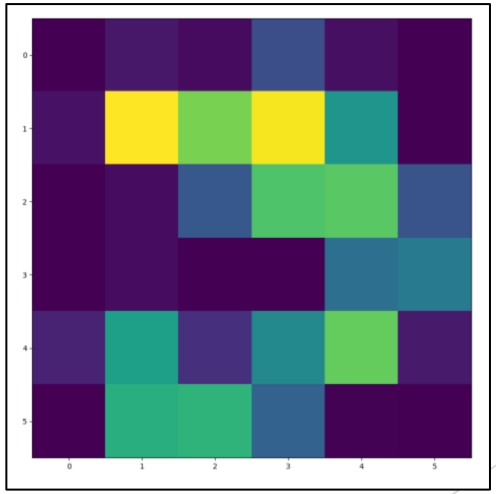

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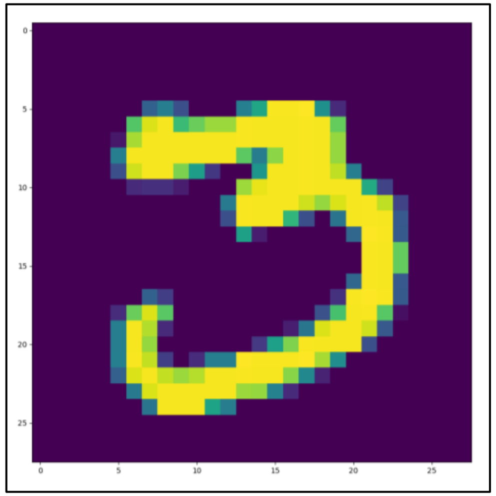

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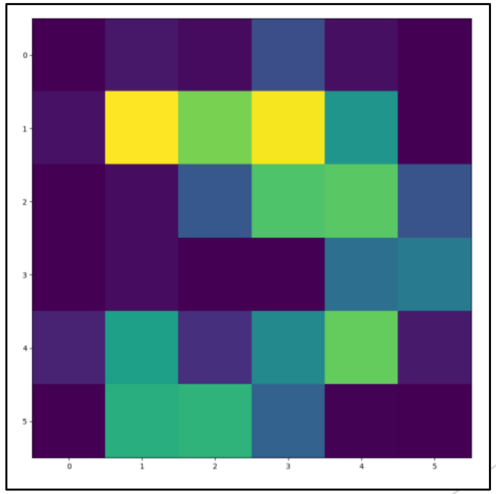

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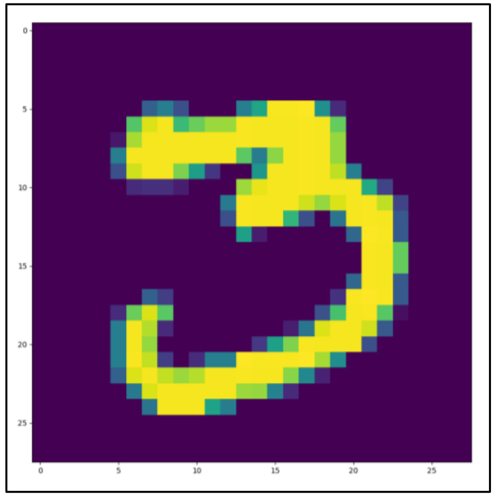

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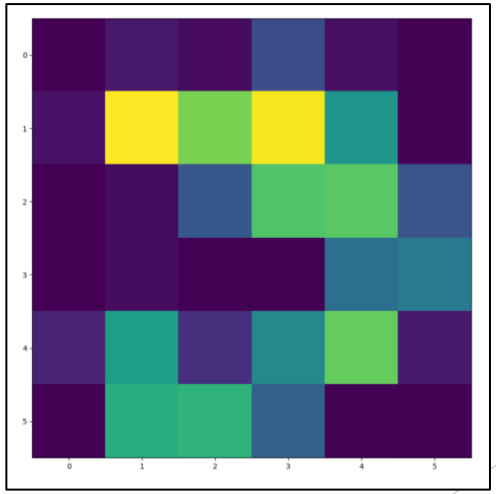

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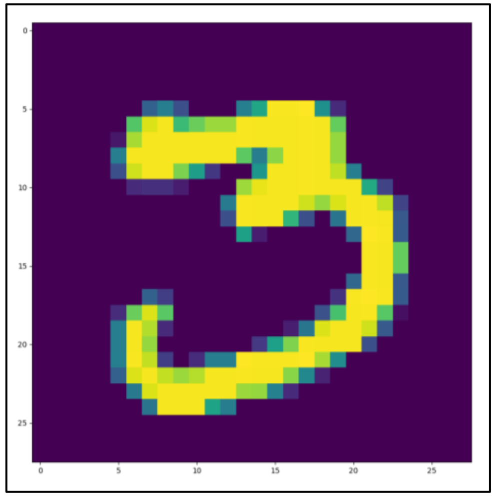

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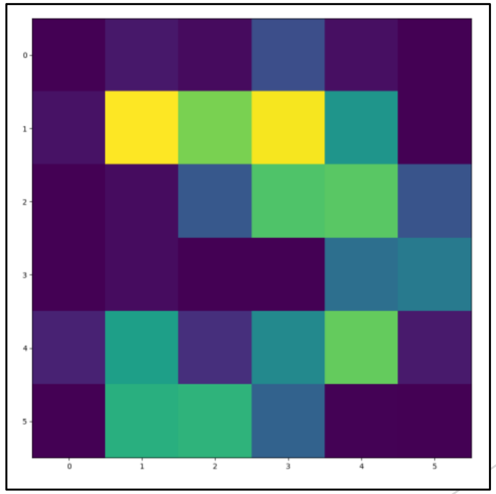

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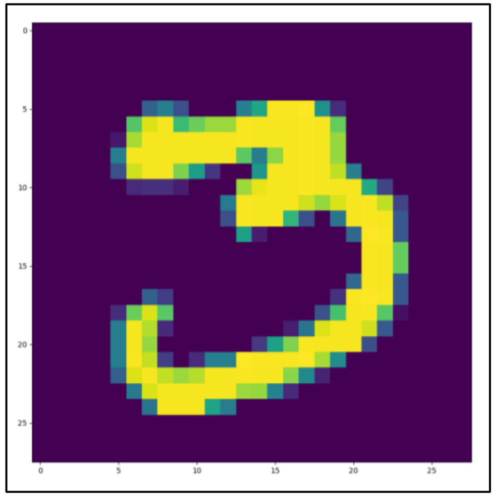

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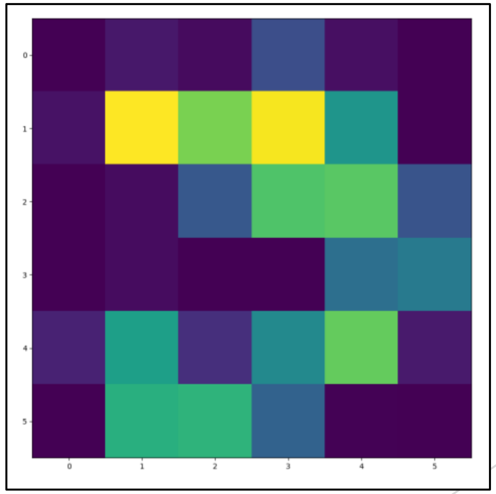

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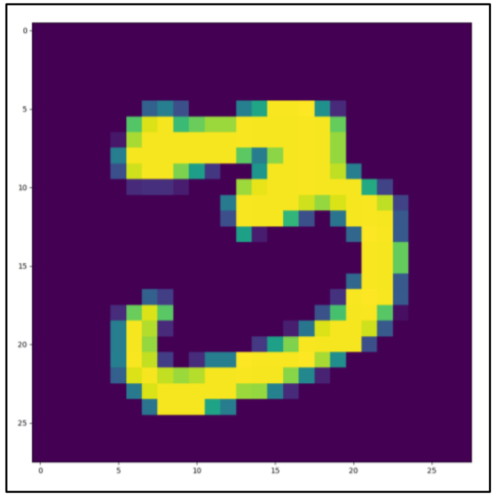

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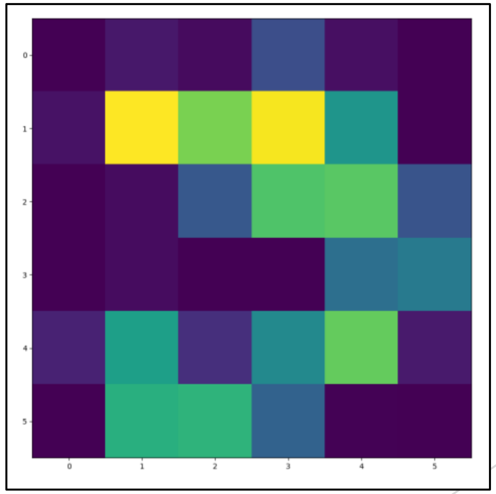

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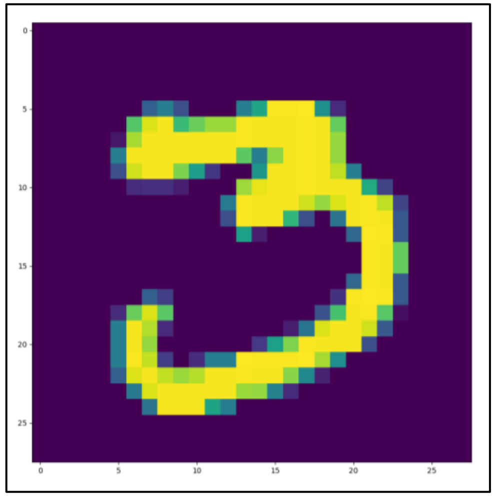

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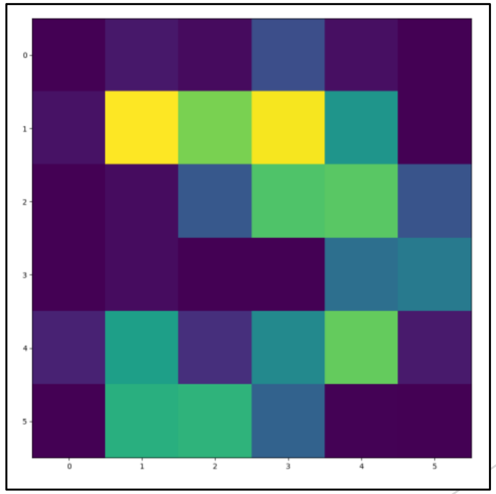

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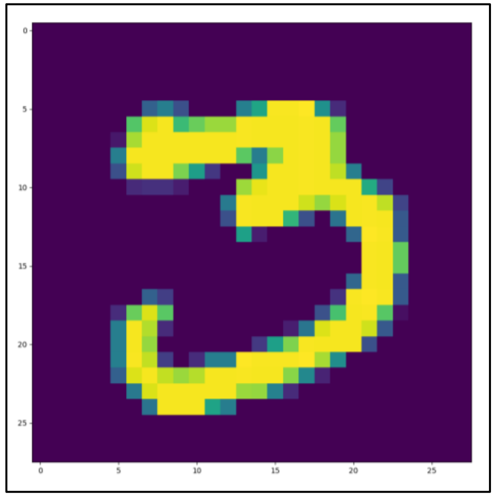

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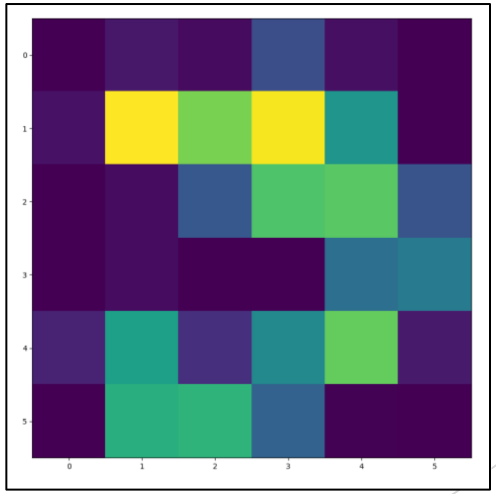

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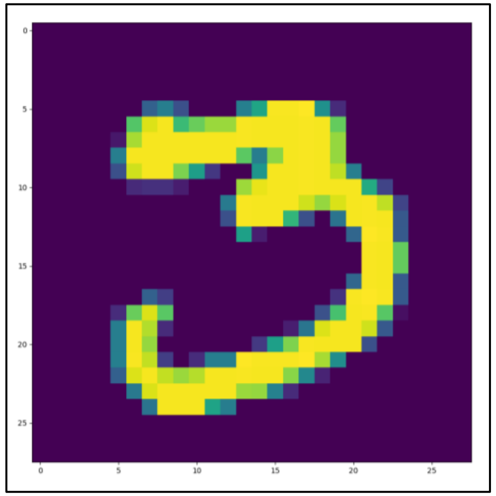
  - Remove the corner pixels and flatten the image into a 1D array (6x6 -> 32x1)



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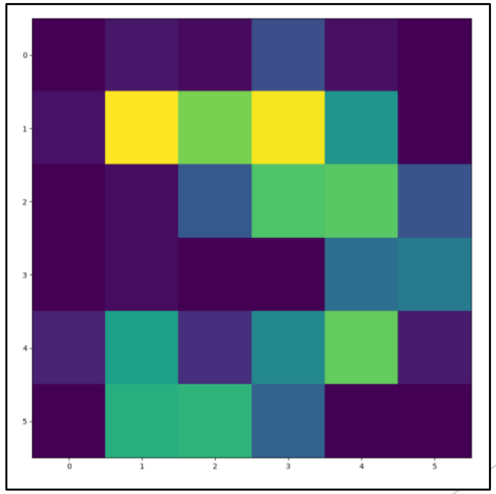

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DBN Training Implementation Details

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- Adachi & Henderson 2015 tested DBN models trained with 1 pre-training iteration to 50 pre-training iterations

	Adachi & Henderson 2015	This Project
Programming Language	Matlab	Python 3
DBN/DNN Implementation	Matlab Deep Learning Toolbox	(confidential)
DBN, DNN structures	32/32/32, 32/32/32/10	32/32/32, 32/32/32/10
Pre-training iterations	1-50 (CPU), 1-50 (QPU)	(confidential)
Trials	10 (CPU), 10 (QPU)	(confidential)
Pre-training learning rate	0.1	(confidential)
Pre-training momentum	0.5 (first 5 iterations), 0.9 (remaining iterations)	(confidential)
Pre-training batch size	6000	(confidential)
Post-training learning rate	0.01	(confidential)
Post-training momentum	0.5 (first 5 iterations), 0.9 (remaining iterations)	(confidential)
Post-training batch size	100	(confidential)

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- Quantum annealing simulation code and D-Wave access library from the D-Wave Ocean SDK

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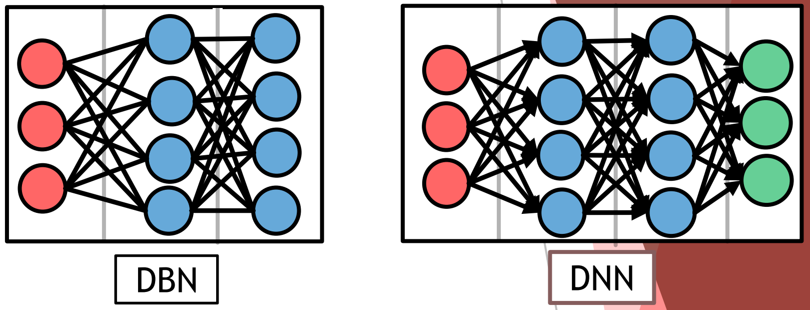
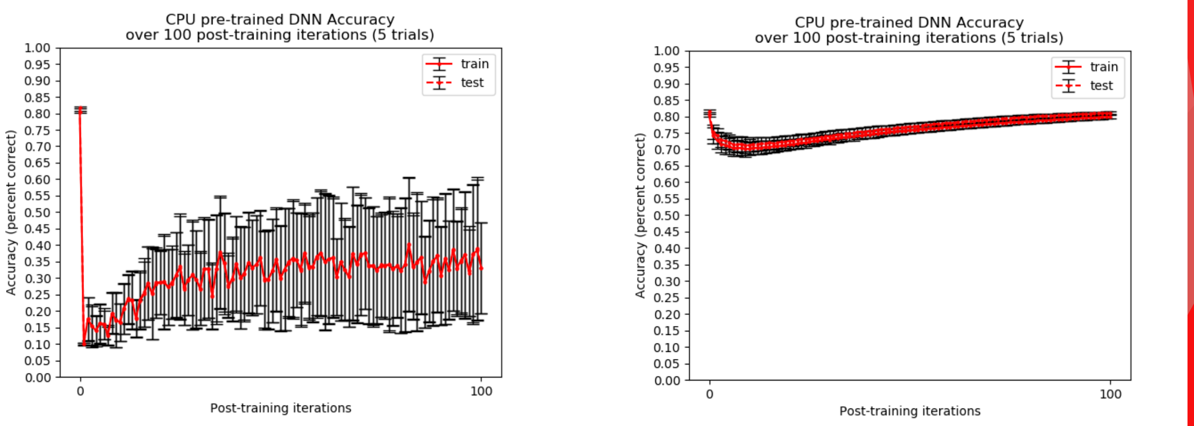
Trials	10 (CPU), 10 (QPU)	(confidential)
Pre-training learning rate	0.1	(confidential)
Pre-training momentum	0.5 (first 5 iterations), 0.9 (remaining iterations)	(confidential)
Pre-training batch size	6000	(confidential)
Post-training learning rate	0.01	(confidential)
Post-training momentum	0.5 (first 5 iterations), 0.9 (remaining iterations)	(confidential)
Post-training batch size	100	(confidential)

DNN post-training Implementation Details

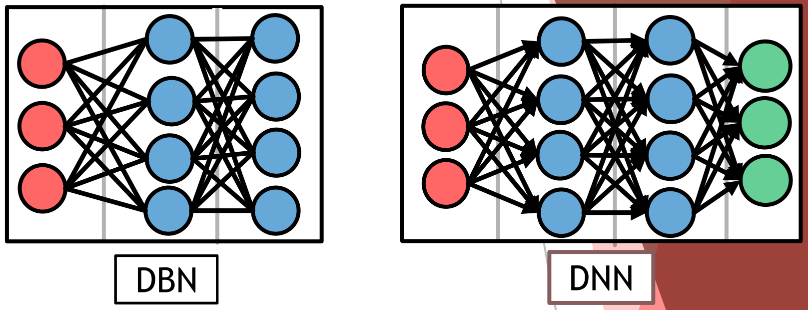


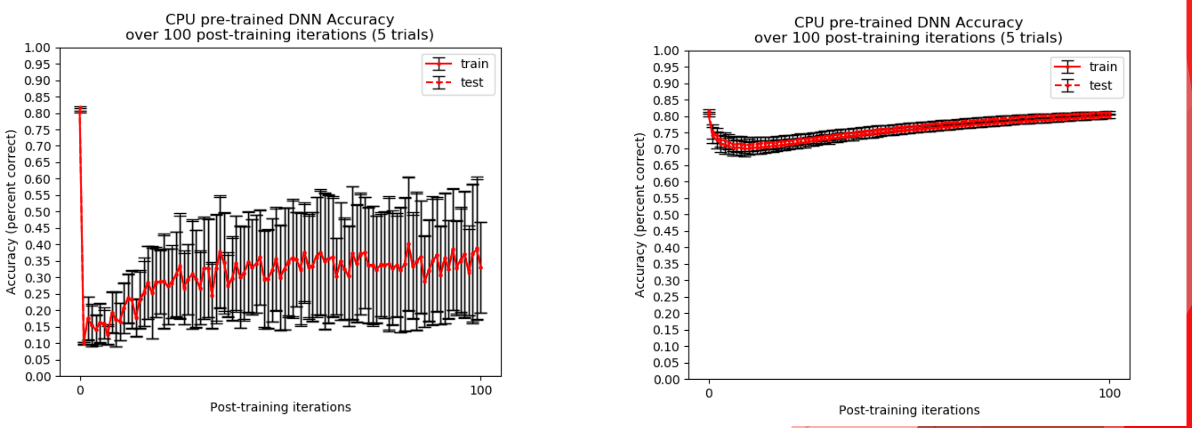


Learning curves for DNN post-training accuracy
(Left) 0 pre-training iterations
(Right) 10 pre-training iterations

DNN post-training Implementation Details

- After DBN models fitted, weights and biases of models extracted to be transferred for use in DNN initialization





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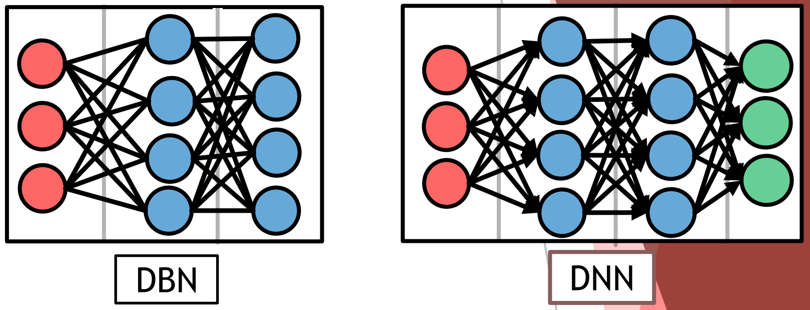
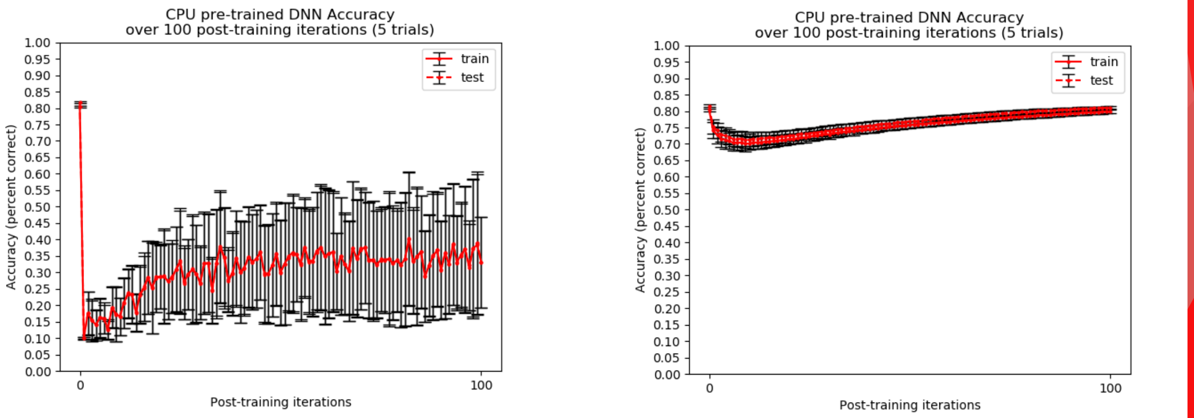
DNN post-training Implementation Details

- After DBN models fitted, weights and biases of models extracted to be transferred for use in DNN initialization
- DNN models trained using SGD with backpropagation





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DNN post-training Implementation Details

- After DBN models fitted, weights and biases of models extracted to be transferred for use in DNN initialization
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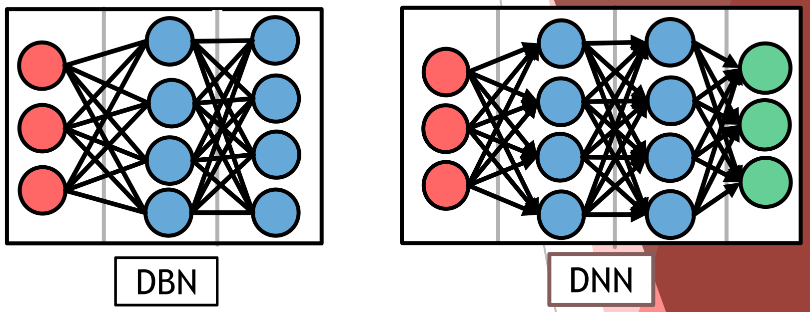
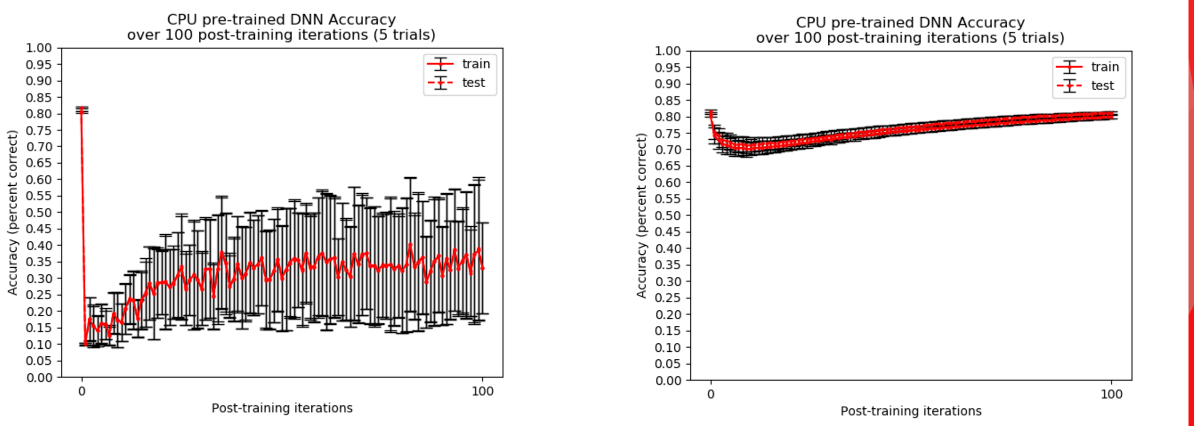
- DNN models' post-training accuracies evaluated against the model's respective training data and against the test set at specified backpropagation iterations





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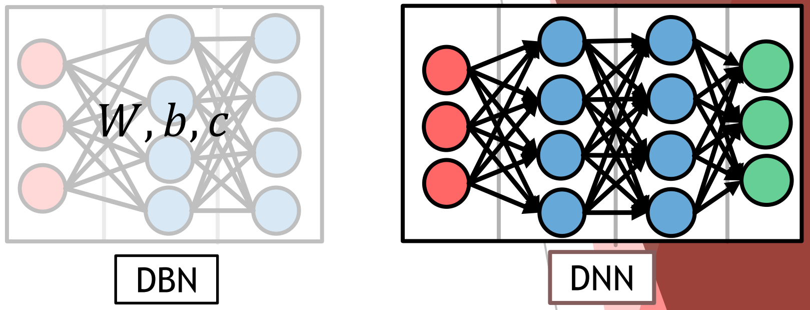

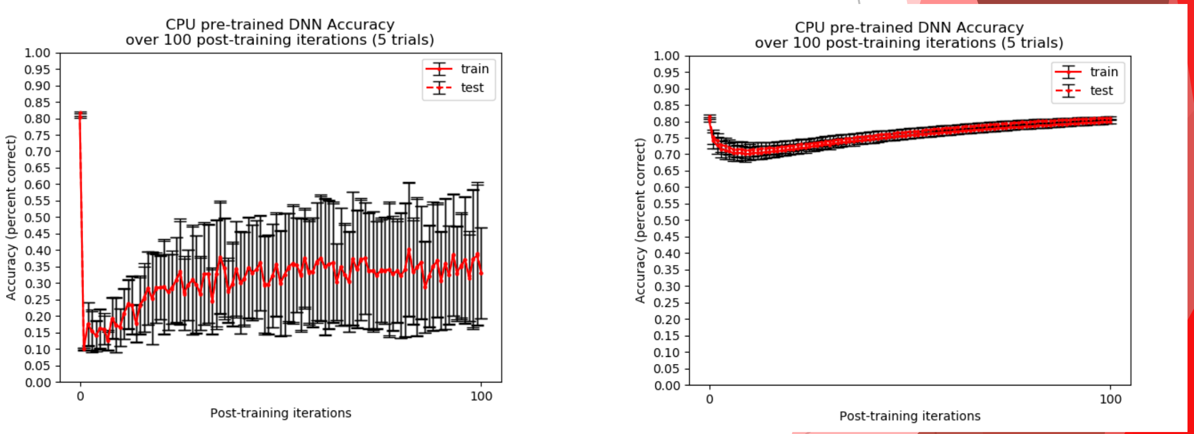

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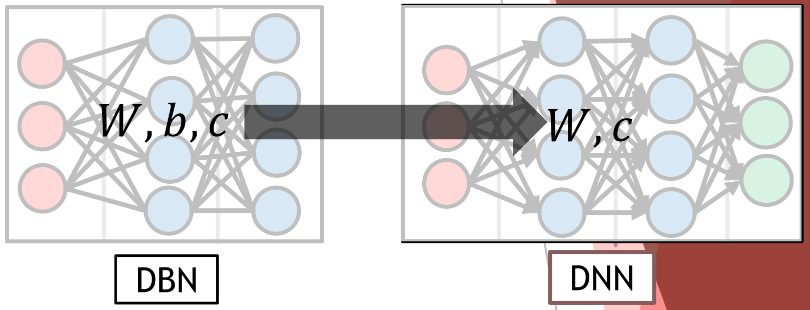

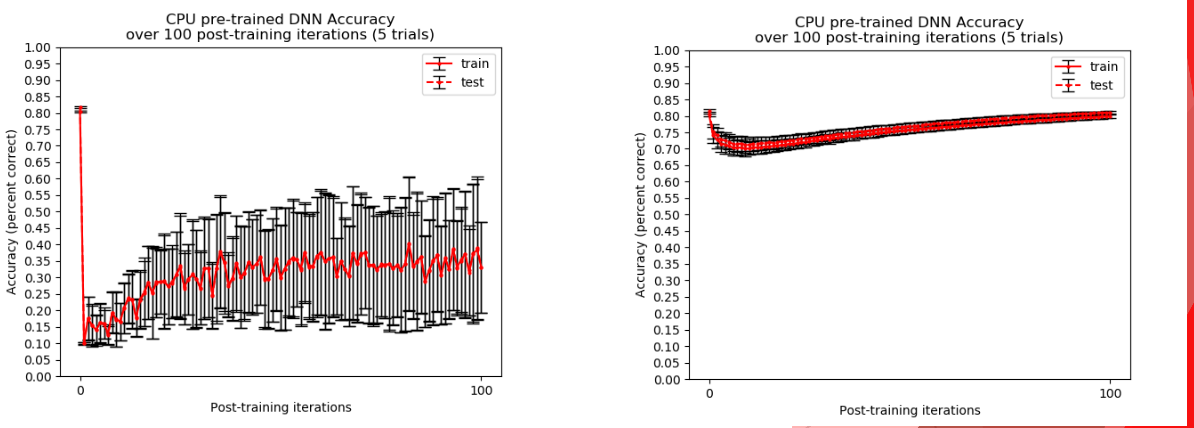

Learning curves for DNN post-training accuracy
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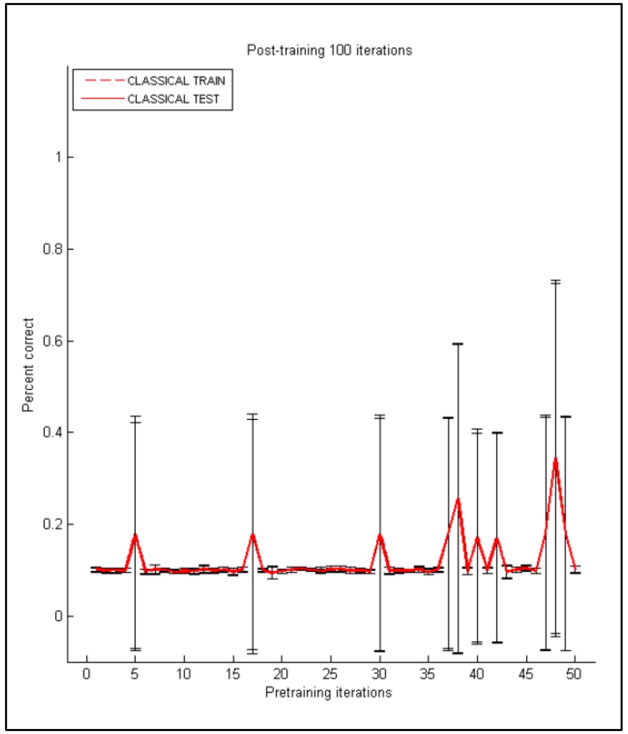
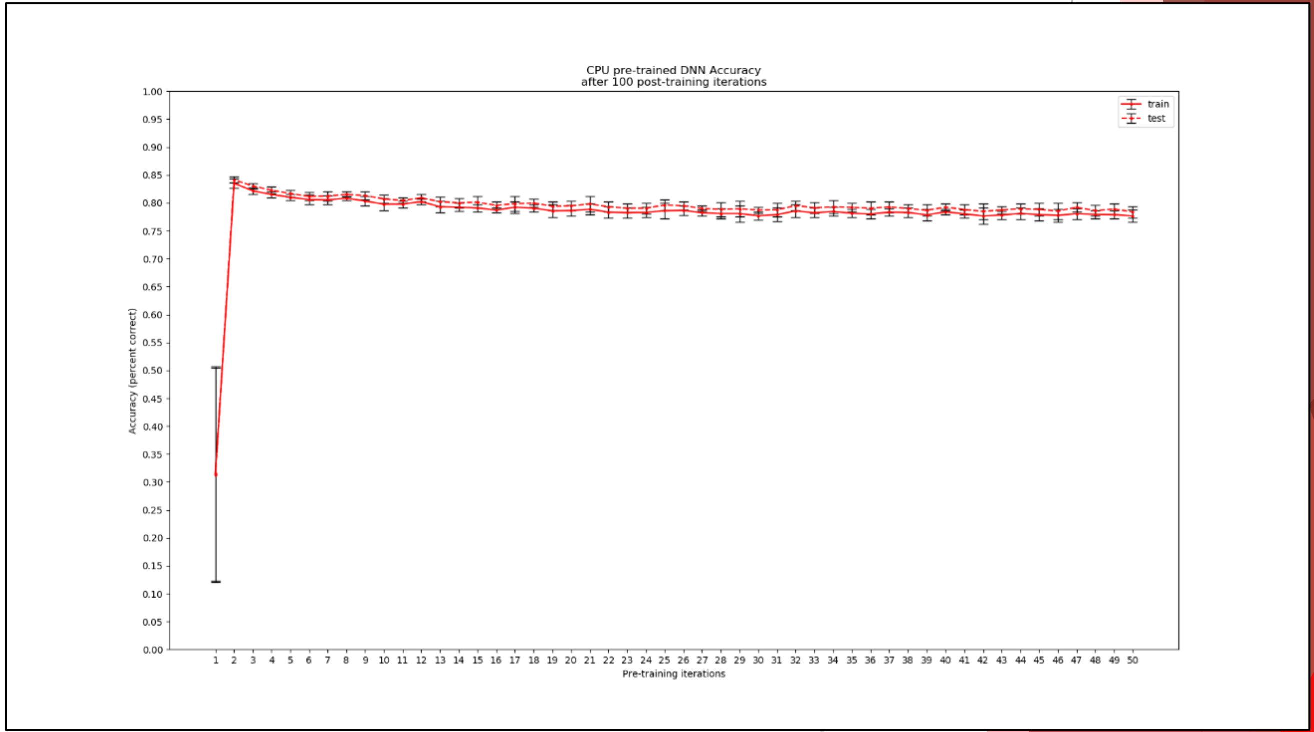
Results

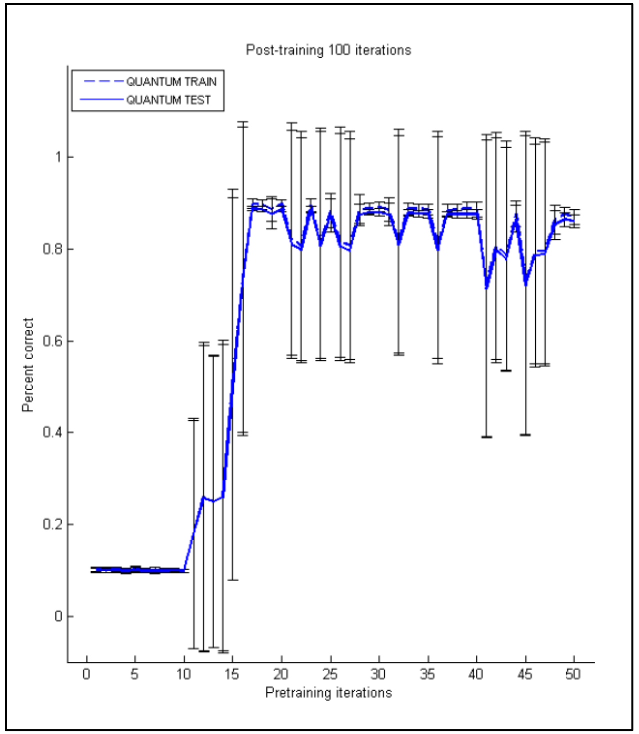
- CPU pre-training, 100 post-training iterations
- (Left: Adachi and Henderson 2015, Right: This project)

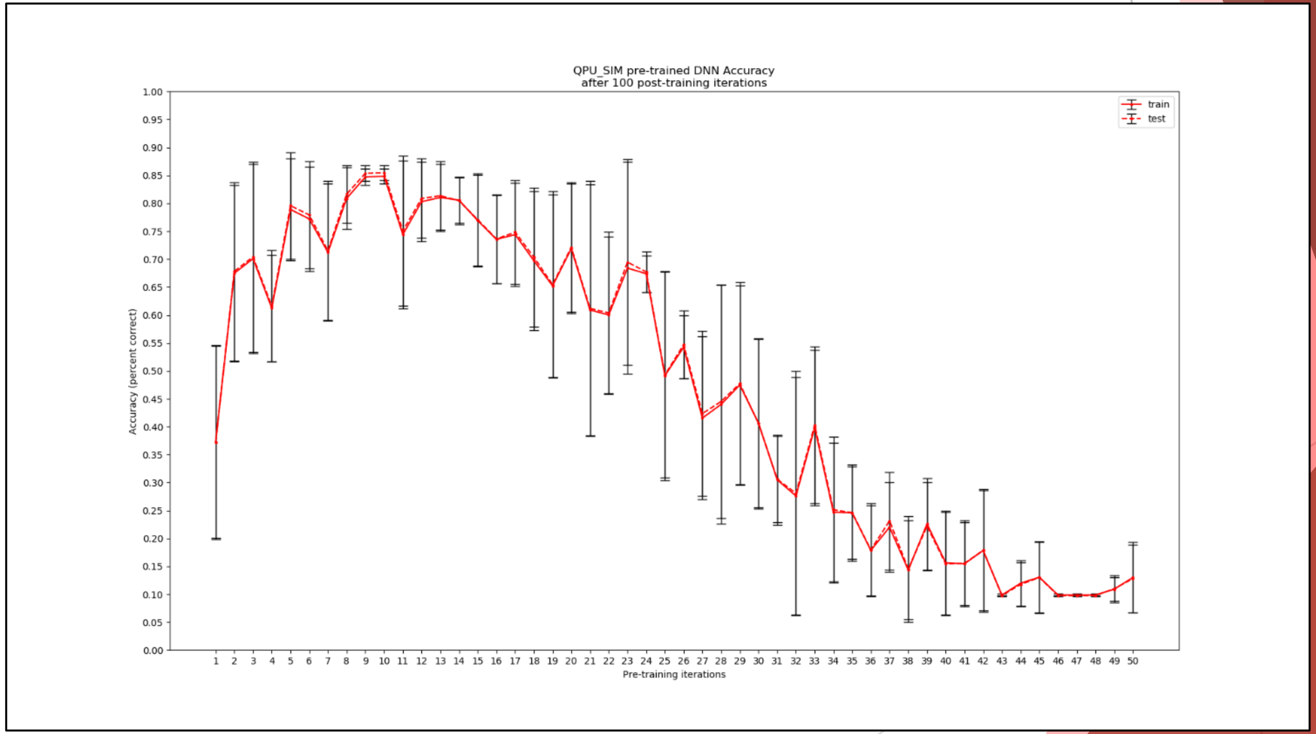




Results

- QPU pre-training, 100 post-training iterations
- (Left: Adachi and Henderson 2015, Right: This project)





Conclusions and Future Developments

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  - Major discrepancies between two sets of results

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References

- [1] Adachi & Henderson, “Application of Quantum Annealing to Training of Deep Neural Networks,” quant-ph. ArXive (2015).
- [2] Erhan et al., “Why Does Unsupervised Pre-training Help Deep Learning?,” Journal of Machine Learning Research (2010).