

# Quantum ML

Week 4 - 2019 AI Inspire

<https://www.youtube.com/watch?v=hWx2Rws3L-A>

<https://www.youtube.com/watch?v=7MPcq8z8jbo>

# Concepts



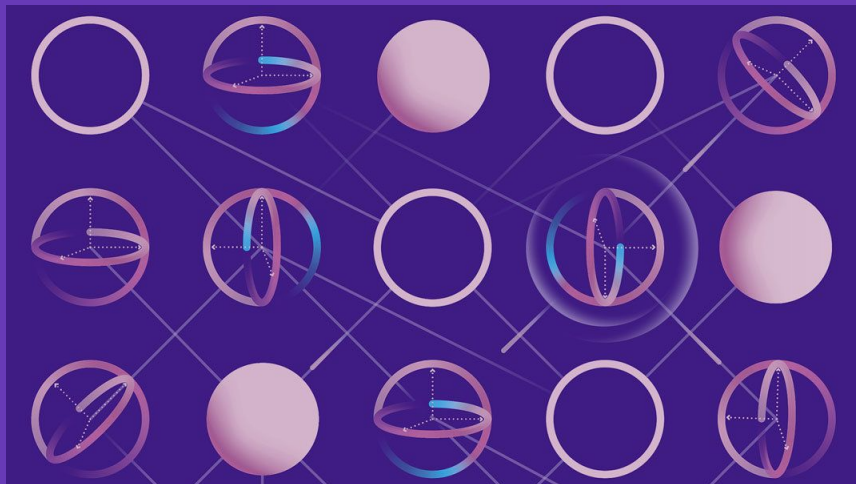
# Recap of Machine Learning

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- Supervised - Input = Labeled training data input → map input to output
- Unsupervised - Input = Unlabeled training data
- Semi-supervised - Input = Small amt of labeled data and large amt of unlabeled
- Reinforcement Learning - Learn to take best course of action to maximize reward in particular environment

# Making the Leap from ML $\rightarrow$ Quantum ML

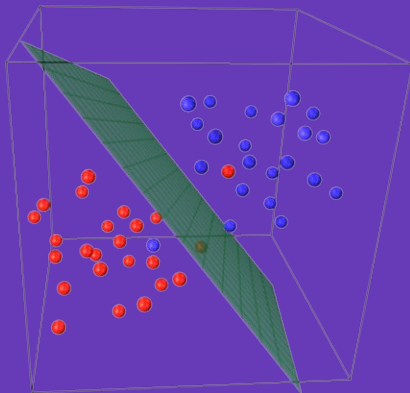
- Classical Machine Learning + Quantum Computing
- Quantum computing  $\rightarrow$  harnesses quantum physics concepts and quantum circuits + qubits & Linear Algebra



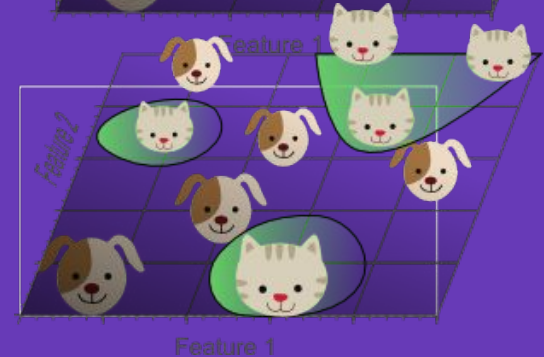
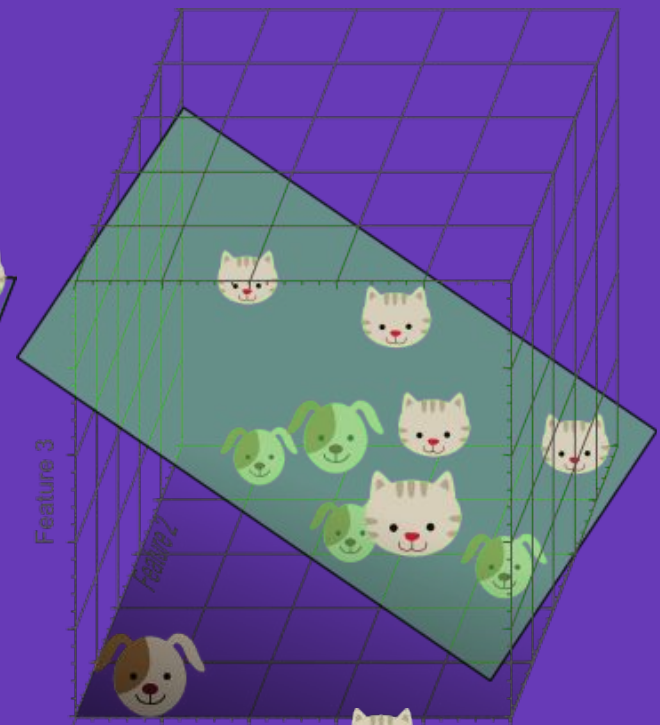
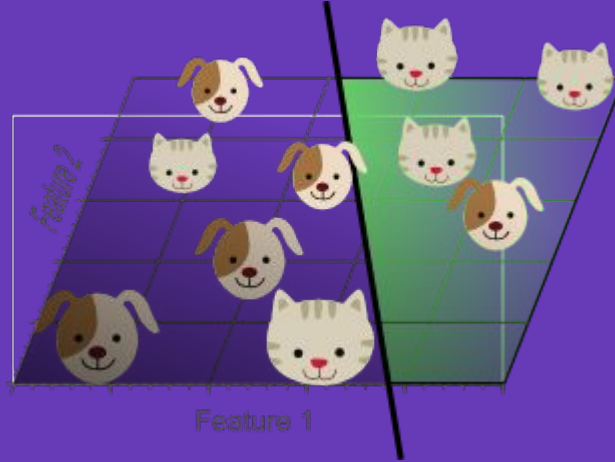
# What is It?

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- Intersection of Quantum Computing and Machine Learning
- Used for nth dimensions (harder to do on classical computer)
- Can classify between multiple diff classes
- Classical computers → easiest for 2 dimensions



# What is It?



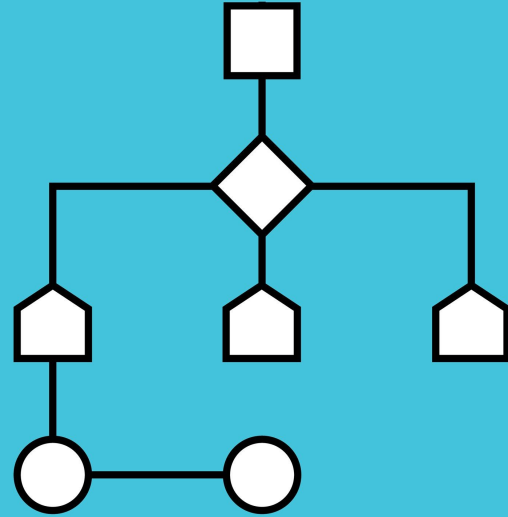
Try to distinguish cats from dogs based on features

Ex - Feature 1 - blue color in dogs and cats

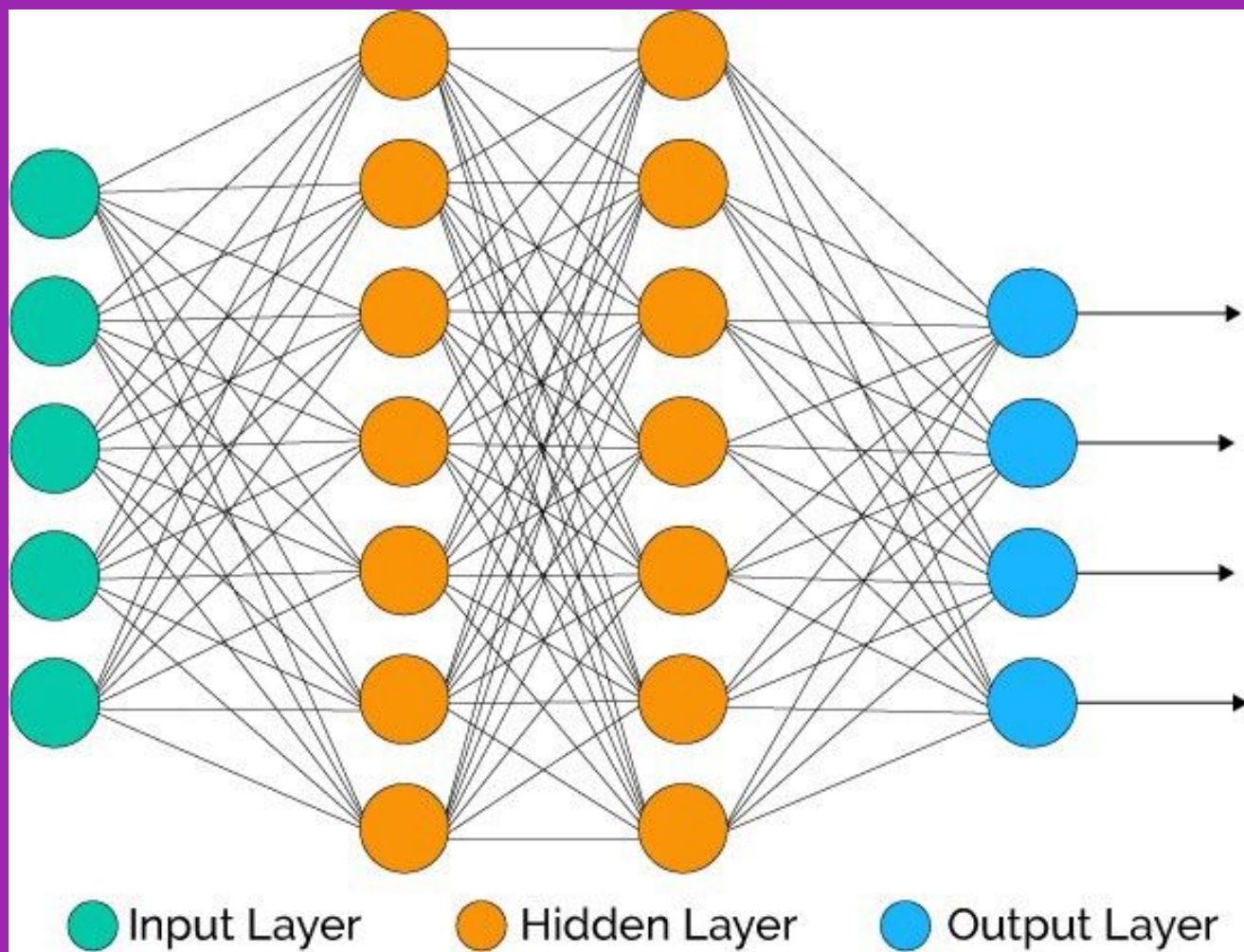
Feature 2 - amt of green color

Feature 3 - amt of red color

# Algorithms



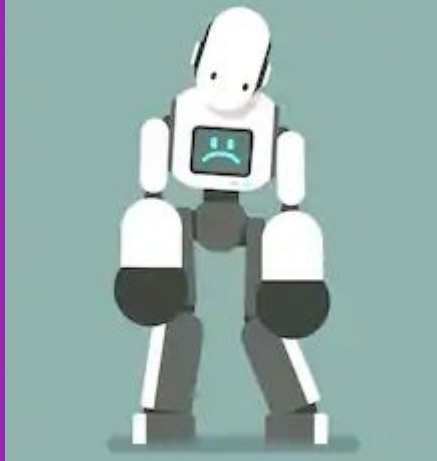




# Challenge of Machine Learning Neural Net

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- A lot of data required to train neural network
- Lot of data → lot of time to make decisions
- Weeks to months amt of time
- Can accelerate training process using Quantum ML

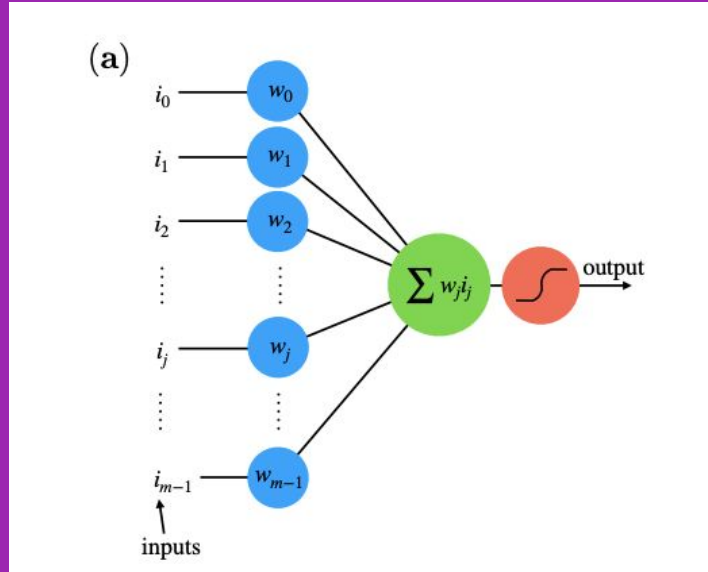


# Quantum Neural Network (QNN)

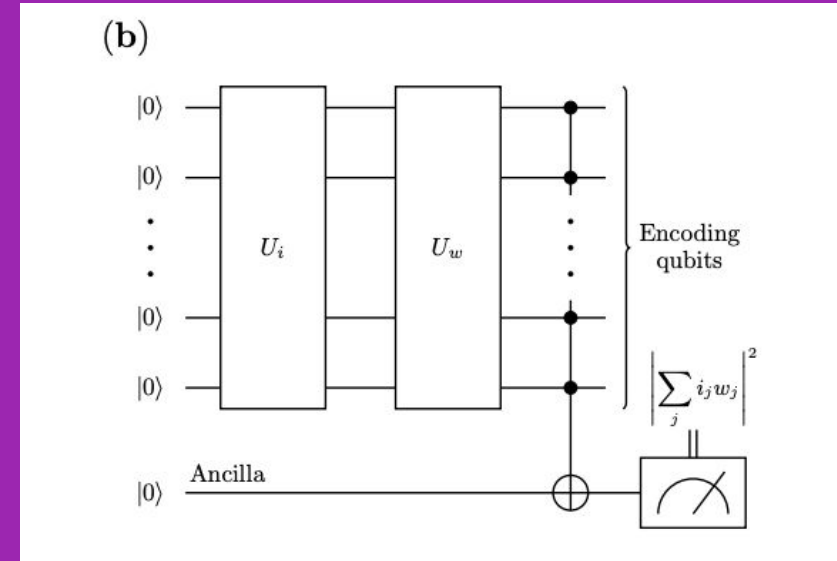
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- Classical neural nets use 1 network → identify patterns
- QNN uses several networks → identify patterns
- Uses quantum physics to use several networks
  - Superposition – possible for qubit to be in many states @ same time
- QNN → stores all possible patterns in a qubit simultaneously

# CNN vs QNN



Output = weighted sum of input vector which passes through sigmoid activation function



1st layer: encodes input vector  $\rightarrow$  quantum states

2nd layer : unitary transformations on input (weight vector)

Output : Ancilla qubit (stores entangled state)













# QNN Advantages

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- Large memory capacity
  - Exponential
- Faster learning
- More stable + reliable
- Able to process much faster



# QNN

states		$ \uparrow\uparrow\rangle$	$ \uparrow\downarrow\rangle$	$ \downarrow\uparrow\rangle$	$ \downarrow\downarrow\rangle$	coherent superposition	
configurations						$\frac{1}{2}( \uparrow\uparrow\rangle -  \uparrow\downarrow\rangle -  \downarrow\uparrow\rangle -  \downarrow\downarrow\rangle)$	
						$\frac{1}{2}(- \uparrow\uparrow\rangle +  \uparrow\downarrow\rangle +  \downarrow\uparrow\rangle -  \downarrow\downarrow\rangle)$	
						$\frac{1}{2}( \uparrow\uparrow\rangle -  \uparrow\downarrow\rangle +  \downarrow\uparrow\rangle +  \downarrow\downarrow\rangle)$	
		$ \uparrow\rangle = \text{"up"} \quad  \downarrow\rangle = \text{"down"}$					

Embedding neurons within qubits

Choosing good neural net is important → performance

STORING ALL POSSIBLE PATTERNS IN QUBITS  
SIMULTANEOUSLY!!!!

QNN of 4 neurons and 2 qubits

Each qubit is represented by a state (up spin or down spin)

Each neuron → associated with state of system

on neuron = + sign in superposition, off = - sign

System existing in combination of states

# QNN Using Hopfield Network

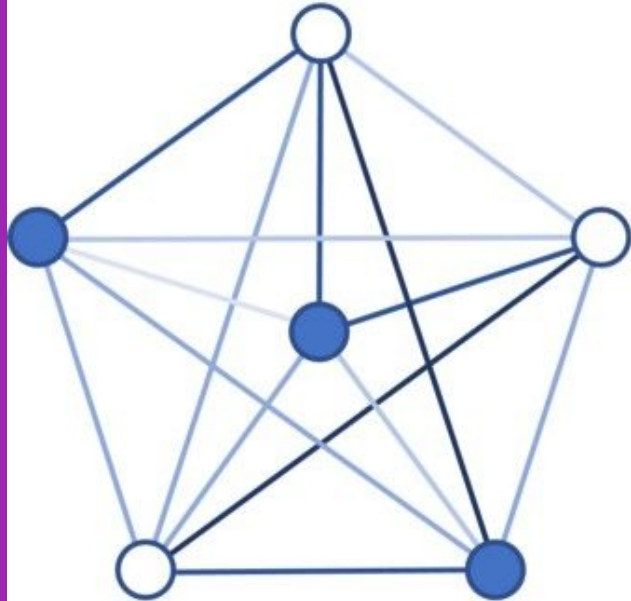
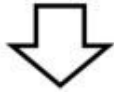
## ➤ Hopfield network

- Type of recurrent neural network
- All neurons are connected to each other
  - Each node can't be connected to itself
- Can change weights between different neurons
- Different configurations of neurons with altering diff weights → diff patterns
- Objective - Hopfield network has diff patterns in memory & want to load new patterns in memory which are most similar to current ones

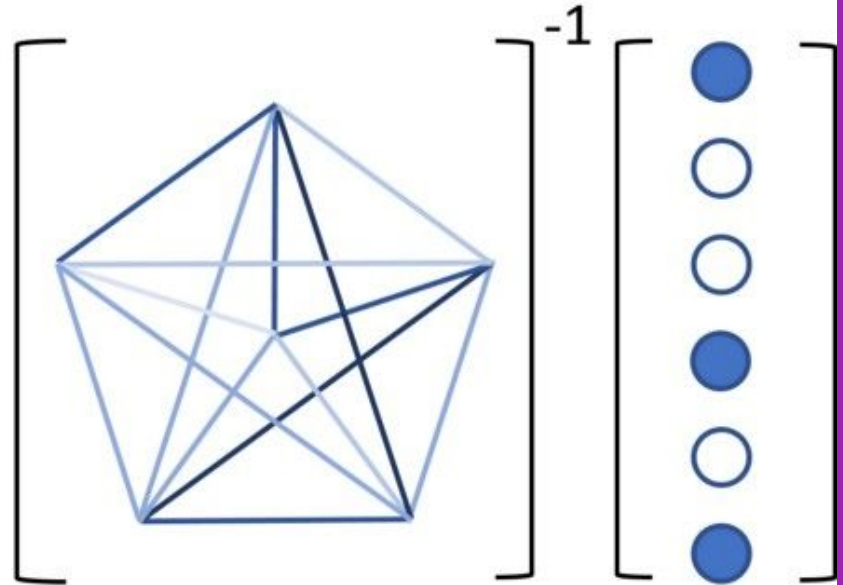
## ➤ How to update network (update weights so output becomes closer to actual output) - **Classical Method**

- Continuously pick neurons and look at the weights between the other nodes it's connected to
- Update each neuron
- Keep on updating till get error to be close to 0, approach finite value asymptotically

pattern



Hopfield network



matrix inversion processing



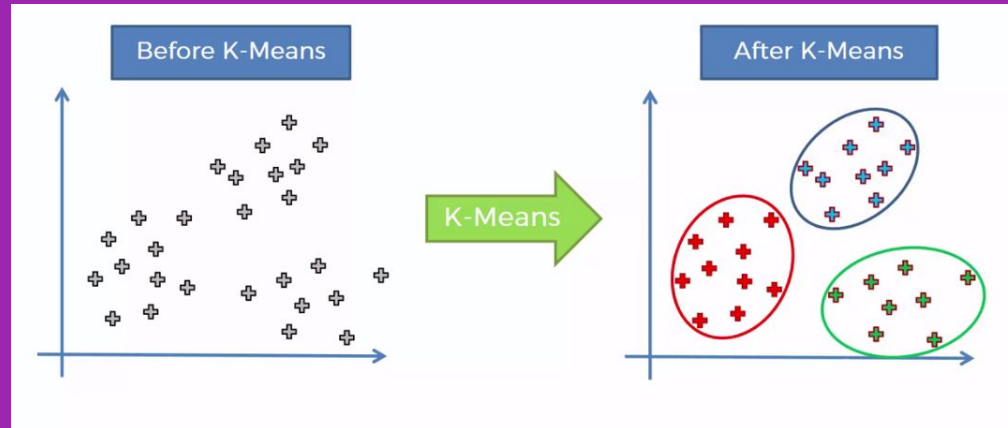
# QNN Using Hopfield Network

## Procedure -

1. Matrix contains weights between all of the neurons in Hopfield network
  - a. Run in 1 step - INVERT matrix (weights needed to come close to actual value happens through inverting matrix)
2. To invert matrix  $\rightarrow$  HHL algo (solve linear system of equations using inverse)  $\rightarrow$  uses Hamiltonian simulation of matrix (quantum Hebbian learning algo)
3. Perform quantum Hebbian learning
  - a. Continuously swaps diff qubit banks which have memory patterns
  - b. Swapping diff qubits in quantum Hebbian learning  $\rightarrow$  “trains the network”

# ML Clustering Algo

- Divide input into  $k$  clusters
- Based off of distance measure between centroids of each cluster (initially randomly assigns centroids and gets better value over iterations)
- Classical k-means algo



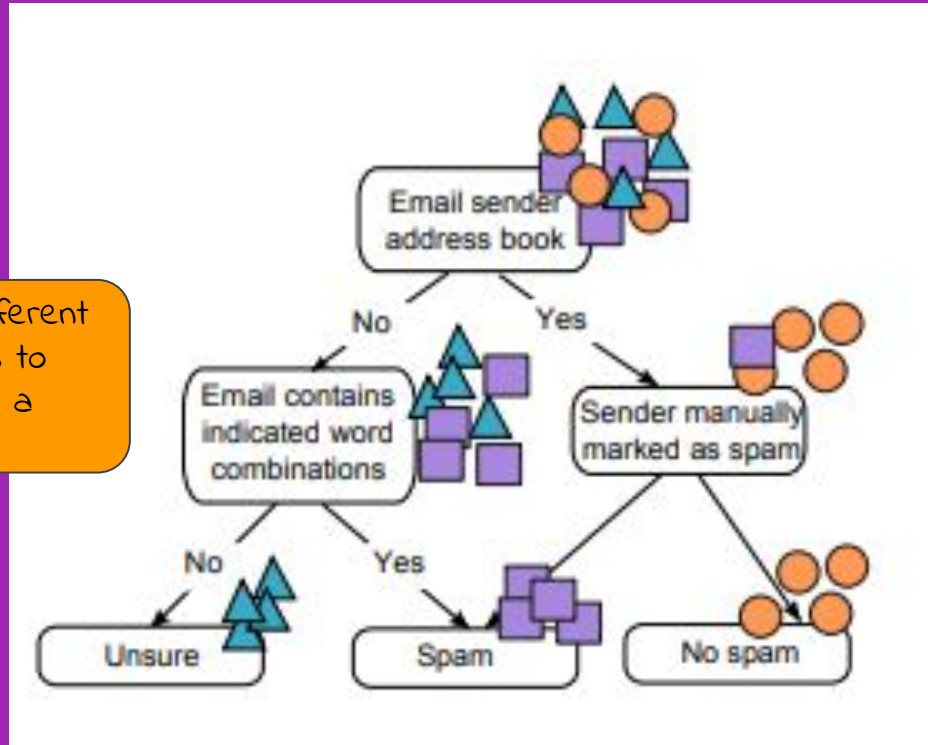
# Quantum Clustering Algo

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- Function calculates dist between 2 states
- For every cluster
  - Calculates summation of distances from each state to other states
  - Quantum state of system can be in quantum superposition → existing in several states @ once
    - Represented as vector → linear algebra needed to compute distances
- Finds the minimum summation
  - Minimum summation = median for cluster

# ML Decision Tree

Split data based on different characteristics/features to reach a consensus with a question



# ML Decision Tree Entropy

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- Entropy = amt of disorder
- Most entropy/disorder in beginning of decision tree
- As you go further down tree and more branches form → less entropy
  - Classes of objects becoming more defined
  - Easier to classify
  - Less entropy/disorder
- Objective - decrease entropy after each cut → if not decreasing, need to split from diff feature/characteristic or stop branch
  - Continuously partitioning/splitting data
  - Least # of branches
  - Start off with broader questions → more specific
- Decision trees use Shannon entropy

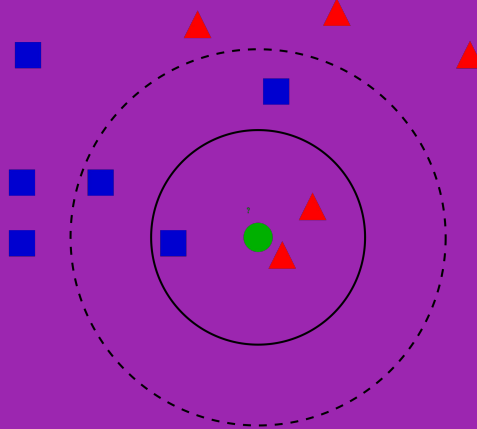
# Quantum Decision Tree Algo

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- Von Neumann Entropy
  - Quantum Mechanics concept for Quantum ML decision trees
  - Parallel to Shannon's entropy used for Classical ML trees
- Quantum decision tree has not actually been constructed yet
- Algorithm still in theory
  - New type of entropy is similar to entropy used in decision tree
  - Harnesses quantum mechanics

# ML K Nearest Neighbors

- Given input, first identify what  $k$  is
- Start from 1st training point and calculate distances from one point to others
  - Sort these distances
  - Identify which distances are the least from the particular training point
- Iterate this process for all training points



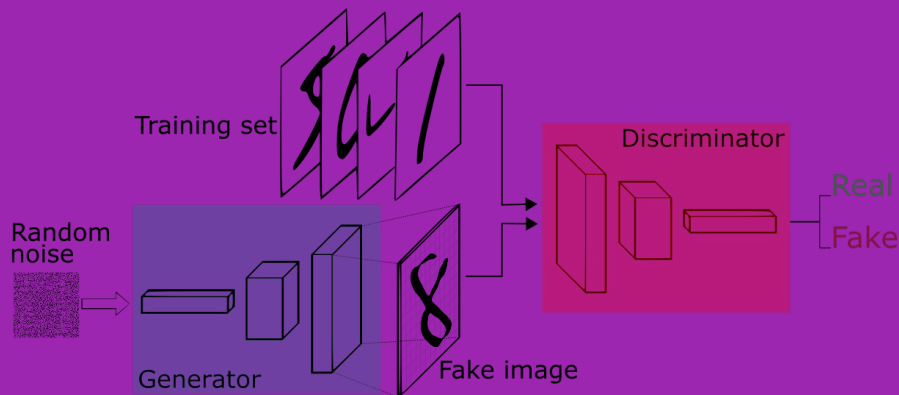
# Quantum K Nearest Neighbors Algo

- Objective - calculate distance between quantum states
  - Once distance is calculated, neighbors can be easily determined
- Classical Euclidean distance → Distance between quantum states (rep as vectors)
- Quantum Swap Test
  - Finds the similarity measure between 2 quantum states using Hadamard logic gate in circuit which puts state in superposition (prob that one state can be transferred to other state after imposing superposition = overlap)
- Overlap of 2 states
  - Shows how close 2 states are to each other
    - Probability 1 state will be exactly like other state
      - 0 = no overlap, 1 = full overlap
  - Obtain overlap of 2 states through quantum swap test
- Obtain distance between 2 states from quantum swap state and fidelity/overlap



# ML Generative Adversarial Network (GAN)

- Unsupervised model using supervised loss function
- 2 competing neural networks
  - Generative and Discriminator
- Great model which solves issue of not having enough data in real world cases → generates own data and gets trained from that
  - Still several challenges of GAN



# ML Generative Adversarial Network (GAN)

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- Generator neural network creates fake images from input vector
- Discriminator network learns to distinguish between the real and false images (real images taken from dataset)
  - Discriminator returns diff prob of each image being real (1 = real and 0 = fake)
- Cop-counterfeiter analogy
  - Counterfeiter learning to pass fake notes and cop is also in training as is able to start distinguishing

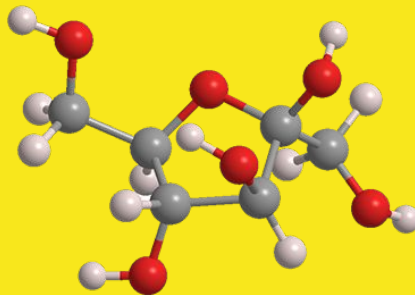
# Applications



# One Application of Quantum ML

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- Classify atoms
- Hard to simulate on classical computers
- More atoms added → molecule becomes more complex
  - Number of interactions between atoms in molecule grow very fast
- Can help with designing new chem compounds
- Discovery of drugs → solve diseases which can't be cured



# Some other application areas

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- More powerful pattern recognition
- Much faster classification
  - Higher dimensions, could be too complex for classical computer
- Developing new types of wearable technologies and materials

# Python

# PennyLane - Python Library

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- Mainly for Quantum Machine Learning
- Compatible with several diff ML libraries
- Optimization + ML tools
- Incorporate quantum circuits
- Hybrid computation
  - Enables both classical and quantum worlds to work together seamlessly



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