Quantum Machine Learning: Opportunities and Challenges

EE350 Technical Communication

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Outline

Machine Learning

- Machine Learning (ML) is the practice of estimating models that make predictions on 'new' data using available data.
- Helpful when the actual model is very complex and no known algorithms can discover such model or they take large amount of time or other resources.

Machine Learning Paradigms

- Supervised ML
  - Classification
    - Categorical (qualitative)
    - Numerical (quantitative)
  - Regression
- Unsupervised ML
  - Clustering
  - Association
- Semi-Supervised ML
- Reinforcement Learning

Issues with ML

- Lack of good quality data sets.
- Possibilty of errors e.g., underfitting or overfitting possible.
- Result are sensitive to small pertubations.
- Safety and Privacy concerns exists.
- Lack of explainability of model.
- Slow process. Training large data sets eates up time.

Quantum Mechanics for Quantum Computation

- A *qubit* is the fundamental data unit of a quantum computer.
- A qubit $|\psi\rangle$ coexists in the states $|0\rangle$ and $|1\rangle$.
- Physical Interpretation

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle. \tag{1}$$

- $|0\rangle$ and $|1\rangle$ are unit vectors and form an orthonormal basis.

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Definition (Inner Product)

$$\langle\psi|\varphi\rangle = \begin{bmatrix} \alpha^* & \beta^* \end{bmatrix} \begin{bmatrix} \gamma \\ \delta \end{bmatrix} = \alpha^*\gamma + \beta^*\delta$$

Postulates of Quantum Mechanics

Definition (Hilbert Space)

A vector space with distance function and inner product among it's elements.

Definition (State Space)

The Hilbert space corresponding to an isolated physical system.

Definition (State Vector)

The state of the system.

Postulate (**State Space**)

The state vector can be completely represented by a unit vector in the state space.

Postulates of Quantum Mechanics

Definition (Hermitian operator)

A Hermitian operator H is its own Hermitian conjugate, i.e $H = H^*$.

Definition (Observable)

A Hermitian operator $\mathcal{O}$ which describes the projective measurement. It acts upon the state space of the system to be measured and is represented as

$$\mathcal{O} = \sum_{\lambda} \lambda P_{\lambda}$$

and P_{λ} is the *projector* with eigenvalue $\lambda \in$ eigenspace of $\mathcal{O}$.

Postulates of Quantum Mechanics

Definition (Unitary Transformation)

A tranformation that preserves inner product. So, a unit vector remains a unit vector after the tranformation. It is denoted by U and it satisfies

$$U^* U = UU^* = I.$$

Postulate (**Measurement**)

A measurement on $\mathcal{O}$ will result in the eigenvalues λ with the probability of collapsing to λ is

$$p_\lambda = \| P_\lambda \langle\psi| \|^2 = \langle\psi|P_\lambda|\psi\rangle .$$

resulting in the irreversibly collapse of the state of system to

$$\frac{1}{\sqrt{p_\lambda} P_\lambda \langle\psi|}.$$

Postulates of Quantum Mechanics

Postulate (Evolution I)

The system evolution is governed by the Schrödinger's equation

$$H \langle \psi(t)| = i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle \psi(t)| .$$

Postulate (Evolution II)

If $\langle \psi_0| , \langle \psi_1|$ describes the state of system at times t_0, t_1 respectively then the evolution of system depends only on t_0 and t_1. It is given by

$$\langle \psi_1| = U \langle \psi_0| .$$

So far, we have studied one-qubit systems. For multi-qubit systems we introduce the following notation.

Postulates of Quantum Mechanics

Definition (Tensor Product (aka Kronecker Product))

For a given m, n dimensional vector spaces V, W. The tensor product of V with W (denoted by $V \otimes W$) is an mn dimensional vector spaces with elements are linear combinations of tensor products $\langle v| \otimes \langle w|$.

We can also define the tensor product of linear operators A, B over vector spaces V, W as

$$(A \otimes B)(\langle v| \otimes \langle w|) = A \langle v| \otimes B \langle w| .$$

Postulate (Composition)

For n isolated systems with states $\langle \psi_0| , \langle \psi_1| , \ldots , \langle \psi_{n-1}|$, the state of the composite system is given by $\langle \psi_0| \otimes \langle \psi_1| \otimes \cdots \langle \psi_{n-1}|$

Quantum Machine Learning (QML)

Quantum-Assisted Machine Learning (QAML)

- Quantum Models *not feasible* in near future.
- A near-term future quantum device will contain 100-1000 qubits.
- Possible applications
  - Hard and out of scope problems for ML. E.g., generative models for semi-supervised and unsupervised ML
  - Datasets with quantum-like connections, turning quantum computers absolutely necessary. E.g., cognitive sciences
  - Hybrid algorithms with a difficult execution step for ML pipeline.

Opportunities in Quantum-Assisted Machine Learning

Unsupervised Learning - Quantum Devices for Sampling

- Incredible amount of unlabelled data available.
- There is a need to extract patterns within such data
- Scientists do not always know what patterns look for
- A need arises for a machine which is capable of extracting order from disorder.

Generative Models

- Generative Model can learn the joint probability among the variables.
- If this is achieved, similar data as the training set can be generated.
- Positive results for high-dimensional data, with correct inference of multi-modal distributions over it.
- The intractable step is computation of expectation values under a complex distribution and this step is a part of each iteration and data point for which Markov chain Monte Carlo (MCMC) techniques are being used.
- Quantum Gibbs distributions are such alternative to MCMC

Cognitive Sciences - Exploiting Datasets

- A quantum model can significantly reduce the computational resources, e.g, memory needed to model a data set.
- Real-life data sets where quantum model is simple compared with classical models must be identified.

Cognitive Sciences - Exploiting Datasets

The Two-Stage Gambling Paradigm

- In the first stage, people were required to gamble. If they win they get x amount of money, if they lose they lose y amount of money (both are equally likely).
- Before learning about the results, participants were asked whether they will 'plan' to gamble again (if they win and if they lose).
- Then after learning the first stage results, final decision was made about playing the second stage was made.

Gamble		Choice Proportions			
Win	Loss	Plan Win	Plan Loss	Final Win	Final Loss
0.8	1	0.25	0.26	0.2	0.35
0.8	0.4	0.76	0.72	0.69	0.73
2	1	0.68	0.68	0.6	0.75
2	0.4	0.84	0.86	0.76	0.89

Table: The Two-Stage Gambling Paradigm[1]

[1] J. Busemeyer, Z. Wang, and R. Shiffrin, "Bayesian model comparison favors quantum over standard decision theory account of dynamic inconsistency," Decision, vol. 2, pp. 1–12, 01 2015.

The Two-Stage Gambling Paradigm

The Quantum Model

- Using quantum theory, this game has 4 events $\{WA, WR, LA, LR\}$ where $W(L)$ stands for win (lose) in first stage and $A(R)$ stands for accept (reject) the second round.
- The person is actually in a superposition of these states

$$|\psi\rangle = \psi_{WA} |WA\rangle + \psi_{WR} |WR\rangle + \psi_{LA} |LA\rangle + \psi_{LR} |LR\rangle$$

  where $|\psi_{WA}|^2$ is the probability that the person belives he won in the first stage and will accept the second stage.
- The initial state is ψ_0 which has some distribution over these 4 amplitudes.
- *Uncertainty* in the first stage results is solved at the second stage after learning the result. Now that state is $\psi_1 = \psi_W = |1100\rangle$ ($\psi_L = |0011\rangle$) if win (lose).
- The payoffs can be achieved using a unitary matrix which rotates ψ towards the gamble or away from it. The final state is

$$\psi_D = U\psi$$

Challenges in Quantum-Assisted Machine Learning

- Compatibility Issues in Hybrid Tech
- Robustness to Noise
- The Curse of Limited Connectivity
- Complex Dataset Representation

Quantum-Assisted Helmholtz Machine (QAHM)

- A hybrid quantum–classical ML which can potentilly handle real-world datasets.
- Its made of a generator network and a recognition network using the notion of stochastic hidden variables.
- Classification can also be implemented in QAHM.

For Further Reading

- C. L. Franklin De Lima Marquezino, Renato Portugal, *A Primer on Quantum Computing*.
  SpringerBriefs in Computer Science, Springer International Publishing, 1 ed., 2019.
- M. Benedetti, J. Realpe-Gómez, and A. Perdomo-Ortiz, "Quantum-assisted helmholtz machines: A quantum–classical deep learning framework for industrial datasets in near-term devices," *Quantum Science and Technology*, vol. 3, p. 034007, may 2018.
- A. Perdomo-Ortiz, M. Benedetti, J. Realpe-Gómez, and R. Biswas, "Opportunities and challenges for quantum-assisted machine learning in near-term quantum computers," *Quantum Science and Technology*, vol. 3, p. 030502, jun 2018.
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