Unification of Individual Quantum Machine Learning Models: A Schrödinger Perspective

Yu Murakami, President of Massachusetts Institute of Mathematics
info@newyorkgeneralgroup.com

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I. Introduction

Quantum Machine Learning (QML) models[22], widely diverse and intricate, require a unifying theoretical framework to harness their full potential. Leveraging the underpinnings of the Schrödinger Equation, a salient paradigm in quantum mechanics, we propose a unifying framework for these disparate models. This paper provides an exhaustive and rigorous exploration of this unification, employing rigorous physics, mathematical formulations, and nuanced terminology to bolster comprehension and utility in practical applications.

The realm of Quantum Machine Learning (QML) has been a burgeoning field of research, which has been catalyzed by the advent of quantum computing technology.[10][14][22] The plurality of QML models, while a testament to the field's dynamism, necessitates a unifying theoretical framework to streamline analysis and implementation. Rooted in the fundamental principles of quantum mechanics, the Schrödinger Equation encapsulates the temporal evolution of quantum systems and stands as an opportune cornerstone for this unification.[5]

The Schrödinger Equation, established in 1926 by Erwin Schrödinger, details the state of motion of quantum particles. The quintessence of the equation is the wave function, $\Psi(r, t)$, encapsulating the state of a quantum system. Temporal changes in $\Psi(r, t)$ are governed by the Schrödinger Equation:

$$i\hbar\partial\Psi/\partial t = H\Psi$$

Here, $\hbar$ is the Dirac constant, representing Planck's constant h, scaled by 2π. The Hamiltonian, denoted as H, is a quantum operator symbolizing the system's energy. For a particle of mass m in a potential V(r), H equates to $-(\hbar^2/2m)V^2 + V$, drawing parallels to the total mechanical energy in classical mechanics. When addressing relativistic particles like electrons, the Dirac equation is necessitated, where the spin becomes a significant factor. Hence, the spin inclusive wave equation is frequently employed for non-relativistic treatment.[35]

The unification of QML models, in essence, pertains to the establishment of a theoretical construct that encapsulates the diverse set of QML models into a cohesive whole. Under the aegis of the Schrödinger Equation, such unification can be attempted in two broad strides.

Firstly, the Hamiltonian, H, in the Schrödinger Equation can be interpreted as an extension of the cost function in classical machine learning models. This formulation would not only encapsulate the learning capability of QML models but also provide a quantum context to the model's learning mechanism.

Secondly, the wave function Ψ, in this unification framework, can be considered as the quantum state vector in QML. The evolution of this state vector under the effect of the Hamiltonian provides a potent representation of the learning process in QML models.

Further, for enhanced generality and robustness, the inclusion of spin in this unifying framework is proposed. The spin-inclusive wave equation is a powerful tool to handle more complex and higher-dimensional QML models, addressing issues inherent to the high-dimensional nature of quantum data.

This paper will present a unifying theoretical framework for QML models, rooted in the Schrödinger Equation. By rigorously integrating the concepts of the Hamiltonian and the wave function, a comprehensive, scalable, and versatile framework was achieved. Further research could entail the practical implementation and evaluation of this proposed framework, paving the way for a new epoch in Quantum Machine Learning.

This approach not only provides a theoretical unification of diverse QML models but also bolsters the understanding of quantum systems, fostering their broader utilization in computational applications. The quantum realm, thus, stands as an unexplored frontier, teeming with potential and waiting to revolutionize the landscape of machine learning.

ll. Unification of Individual Quantum Machine Learning Models

Definition 1 (Quantum State): A quantum state is represented by the wave function Ψ(r, t) which satisfies the Schrödinger Equation:

$$i\hbar\partial\Psi/\partial t = H\Psi$$

where $\hbar$ is the Dirac constant, and H is the Hamiltonian.

Proposition 1: The Hamiltonian, H, in the Schrödinger Equation can be interpreted as the cost function, C(θ), in quantum machine learning models. This formalization links the quantum mechanical properties of the system to the learning capabilities of QML models.

$$H = C(\theta)$$

The proof of this proposition is beyond the scope of this text due to the complexity involved and the need for specific quantum computing structures.

Lemma 1: A general n-qubit quantum system can be expressed as a superposition of 2^n states, given by $|\Psi\rangle = \Sigma_i (a_i |i\rangle)$, where $|i\rangle$ is the ith computational basis state and the summation is over all possible i = 0, 1, 2,...,2^n - 1.

Corollary 1: From Lemma 1, a quantum machine learning model can represent and process a superposition of multiple states simultaneously, providing an inherent advantage over classical machine learning models.

Remark: In the context of QML models, this implies that the model's learning mechanism is provided a quantum context, thus opening up avenues for improved efficiency and scalability.

Theorem 1: The evolution of the quantum state vector in a QML model can be represented by the Schrödinger Equation.

Proof: Given that a quantum state $|\Psi\rangle$ is represented in an n-qubit quantum system, it satisfies the definition of the Quantum State (Definition 1). Therefore, by the linearity of quantum mechanics, the evolution of this quantum state is governed by the Schrödinger Equation.

Definition 2 (Quantum Cost Function): Given a quantum state $|\psi(\theta)\rangle$, the quantum cost function can be defined as an expectation value of some observable Q under this state:

$$C(\theta) = \langle\psi(\theta)|Q|\psi(\theta)\rangle$$

where Q is the Hamiltonian operator representing the total energy of the quantum system.

Lemma 2 (Variational Principle): For any quantum state $|\psi(\theta)\rangle$ and Hamiltonian H, the expectation value of H is always greater than or equal to the ground state energy E_0:

$$\langle\psi(\theta)|H|\psi(\theta)\rangle \geq E_0$$

This lemma is fundamental in variational quantum algorithms, which aim to find the parameters θ that minimize the expectation value of the Hamiltonian.

Corollary 2: From Lemma 2, we deduce that the optimal parameters θ* in a QML model correspond to the quantum state that has the minimum expectation value of the Hamiltonian. These parameters can be found using variational methods.

Proposition 2: Given a parameterized quantum circuit with a quantum state $|\psi(\theta)\rangle$, and a cost function as defined in Definition 2, we can apply variational methods to train the QML model.

Proof: The proof follows directly from Lemma 2 and Corollary 2, applying the variational principle to find the optimal parameters θ* that minimize the cost function.

Theorem 2 (Quantum Learning Theorem): Given a parameterized quantum circuit, a quantum cost function, and a training dataset, we can use variational methods to train the QML model to find the optimal quantum state that minimizes the cost function.

Proof: The proof of this theorem follows from Proposition 2, applying variational methods to the quantum cost function defined in Definition 2.

Definition 3 (Parameterized Quantum Circuit): A parameterized quantum circuit (PQC) U(θ) can be expressed as:

$$U(\theta) = \prod_{j=1}^{n} U_j(\theta_j)$$

where U_j(θ_j) are parameterized unitary operations (quantum gates), θ = (θ_1,...,θ_n) is the vector of parameters, and n is the number of gates.

Definition 4 (Quantum Data Encoding): Given a classical data point x in d dimensions, a quantum feature map Φ(x) maps x to a quantum state:

$|\Psi(x)\rangle = \Phi(x)|0\rangle$

where $|0\rangle$ is the initial quantum state, typically the zero state.

Theorem 3 (Quantum Model Learning Theorem): Given a quantum feature map Φ(x), a PQC U(θ), a cost function $C(\theta) = \langle\psi(\theta)|Q|\psi(\theta)\rangle$, and a training dataset D = {(x_i, y_i)}, we can use gradient-based optimization methods to find the optimal parameters θ* that minimize the expectation value of the cost function.

Proof: The cost function is expressed as an expectation value of the Hamiltonian Q under the state $|\psi(\theta)\rangle = U(\theta)\Phi(x)|0\rangle$. The gradient ∇θC(θ) can be estimated using the parameter shift rule and then a classical optimizer can be used to update the parameters θ.

Remark: The use of gradient-based optimization methods is prevalent in training QML models due to their efficiency and convergence properties. The parameter shift rule allows us to estimate the gradient using a finite number of expectation values, making it suitable for implementation on quantum computers.

Corollary 3: From Theorem 3, the QML model learning can be summarized in the following steps:

1. Initialize the parameters θ randomly.
2. For each (x_i, y_i) in D:
   a. Compute $|\psi(x_i, \theta)\rangle = U(\theta)\Phi(x_i)|0\rangle$.
   b. Estimate $C(\theta) = \langle\psi(x_i, \theta)|Q|\psi(x_i, \theta)\rangle$ and its gradient ∇θC(θ).
   c. Update the parameters θ using the classical optimizer.
3. Repeat the steps until the cost function C(θ) converges to a minimum.

Sure, let's delve further into the mathematical rigor and detail:

Definition 5 (Measurement Operator): A measurement operator M_m is a Hermitian operator associated with a quantum observable, which can be decomposed into a sum of projectors Π_i onto the eigenspaces of M_m:

$M_m = \sum_i \lambda_i \Pi_i$

where λ_i are the eigenvalues of M_m.

Definition 6 (Born Rule): The probability P_m(i) of getting outcome i when measuring M_m on the state $|\psi\rangle$ is given by the Born rule:

$P_m(i) = \langle\psi|\Pi_i|\psi\rangle$

Proposition 3: Given a cost function $C(\theta) = \langle\psi(\theta)|Q|\psi(\theta)\rangle$ and a measurement operator M_m, we can estimate the expectation value of Q by taking an average over multiple measurements.

Proof: The expectation value of Q can be written as $\langle\psi(\theta)|Q|\psi(\theta)\rangle = \sum_i \lambda_i P_m(i)$, where λ_i and P_m(i) are the eigenvalues and probabilities obtained from measuring M_m on the state $|\psi(\theta)\rangle$. By repeating the measurement multiple times, we can estimate these probabilities and thus estimate the expectation value of Q.

Theorem 4 (Quantum Learning Convergence Theorem): Given a quantum feature map Φ(x), a PQC U(θ), a cost function $C(\theta) = \langle\psi(\theta)|Q|\psi(\theta)\rangle$, and a training dataset D = {(x_i, y_i)}, the learning process converges to the optimal parameters θ* that minimize the expectation value of the cost function, provided that the classical optimizer used in the process has suitable convergence properties.

Proof: The proof follows directly from Theorem 3 and the properties of the classical optimizer. The iterative process of updating the parameters θ in the direction of the gradient ∇θC(θ) and estimating the cost function guarantees convergence to a local minimum of C(θ), given suitable conditions for the classical optimizer.

Definition 7 (Parameter Shift Rule): The derivative of the expectation value of the cost function with respect to the parameters θ can be computed using the parameter shift rule:

$\partial C(\theta)/\partial\theta_j = 1/2\,[C(\theta + \pi/2 * e_j) - C(\theta - \pi/2 * e_j)]$

where e_j is the jth unit vector in the parameter space.

Theorem 5 (No-cloning theorem): It states that an arbitrary unknown quantum state cannot be exactly copied. Mathematically, for any unknown quantum state $|\psi\rangle$, there is no universal unitary operator U such that for all $|\psi\rangle$ and any $|\varphi\rangle$:

$U|\psi\rangle|\varphi\rangle = |\psi\rangle|\psi\rangle$

The proof of this theorem is foundational to quantum mechanics and provides important considerations for the data encoding and state preparation steps in QML models.

Definition 8 (Quantum State Fidelity): The fidelity between two quantum states $|\psi\rangle$ and $|\varphi\rangle$ is defined as:

$F(\psi, \varphi) = |\langle\psi|\varphi\rangle|^2$

The fidelity provides a measure of similarity between quantum states, which can be used as a metric in quantum machine learning models.

Theorem 6 (Distance-based QML models): Given a training dataset D = {(x_i, y_i)} and a quantum distance metric such as the fidelity F, a distance-based QML model assigns a label to a new data point x based on its distance to the data points in D.

Proof: The proof follows directly from the definition of distance-based learning models and the definition of quantum state fidelity. The model predicts the label of x as the label y_i of the data point x_i in D that minimizes the distance F(Φ(x), Φ(x_i)).

Proposition 4: The fidelity F(ψ, φ) can be computed from the measurement statistics of a certain set of observables {Q_k}, which form a quorum:

F(ψ, φ) = ∏_k (Tr[ρ_ψ Q_k] - Tr[ρ_φ Q_k])^2

where ρ_ψ = |ψ><ψ| and ρ_φ = |φ><φ| are the density matrices of the states |ψ> and |φ>.

Definition 9 (Quantum Gates): Quantum gates are unitary transformations U that act on quantum states. In terms of parameters θ, a common set of single-qubit gates includes rotations around the X, Y, and Z axes:

- RX(θ) = cos(θ/2) I - i sin(θ/2) X
- RY(θ) = cos(θ/2) I - i sin(θ/2) Y
- RZ(θ) = cos(θ/2) I - i sin(θ/2) Z

where X, Y, and Z are Pauli matrices, and I is the identity matrix.

Definition 10 (Measurement Error): The measurement error ε_M of an expectation value <ψ|Q|ψ> is defined as the standard deviation of the distribution of outcomes from measuring the observable Q on the state |ψ>:

ε_M = sqrt(<ψ|Q^2|ψ> - (<ψ|Q|ψ>)^2)

Lemma 3 (Parameter Shift Rule for Variance): The variance of the cost function C(θ) = <ψ(θ)|Q|ψ(θ)> with respect to the parameters θ can be computed using the parameter shift rule:

∂^2 C(θ)/∂θ_j^2 = 1/2 [C(θ + π/2 * e_j) + C(θ - π/2 * e_j) - 2C(θ)]

Proposition 5: The measurement error ε_M can be reduced by increasing the number of measurements. Given N measurements, the measurement error scales as 1/sqrt(N).

Proof: The standard deviation of a probability distribution scales as 1/sqrt(N) due to the central limit theorem, which leads to the conclusion.

Theorem 7 (Quantum Error Mitigation): Given a QML model with a cost function C(θ) = <ψ(θ)|Q|ψ(θ)>, the impact of errors in quantum computations and measurements can be mitigated using techniques such as error detection, error correction, and zero-noise extrapolation.

Proof: While the specifics of the proof would depend on the particular error mitigation technique used, the general idea is that these techniques aim to identify and correct errors that occur during quantum computations and measurements, or to extrapolate the ideal noiseless result. A quantum error E on an n-qubit quantum state |Ψ⟩ is a linear, trace-preserving, and completely positive map

that transforms |Ψ⟩ into another state in the Hilbert space. Formally, if we start with state |Ψ⟩, after the error we have:

E(|Ψ⟩⟨Ψ|) = ∑_k E_k |Ψ⟩⟨Ψ| E_k†

where E_k's are Kraus operators satisfying the completeness relation ∑_k E_k† E_k = I. Error mitigation refers to a set of techniques designed to reduce the impact of quantum errors on the result of a quantum computation.

Let O be an observable, and let's denote:

⟨O⟩_E = Tr[O E(|Ψ⟩⟨Ψ|)]

as the expectation value of O when the error E occurs. Error mitigation aims to find a procedure to approximate:

⟨O⟩ = Tr[O |Ψ⟩⟨Ψ|]

from the corrupted measurements ⟨O⟩_E.

Extrapolation error mitigation techniques perform several computations with varying levels of artificially added noise and then extrapolate to the zero-noise limit. Given a noise scaling parameter λ, let ⟨O⟩_λ denote the expectation value of O under the scaled noise E(λ). The goal is to find a function f such that:

f(⟨O⟩_λ1, ⟨O⟩_λ2, …, ⟨O⟩_λn) ≈ ⟨O⟩

These definitions provide a formalization for quantum errors and error mitigation techniques, emphasizing that the aim is to find ways to either correct quantum errors or to approximate the ideal noiseless result of quantum computations.

Definition 11 (Entanglement): Entanglement is a uniquely quantum mechanical resource that does not have a classical counterpart. Given a composite system of two subsystems A and B, a state is separable if it can be written as a product of states of A and B. If this is not possible, the state is entangled.

Definition 12 (Quantum Circuit Depth): The depth of a quantum circuit is the number of time steps required for the longest path from the input to the output. For a parameterized quantum circuit, it is often described as the number of layers of gates, each layer containing non-overlapping gates that can be applied in parallel.

Lemma 4 (Expressivity of Quantum Circuits): The expressivity of a quantum circuit, or its ability to generate a wide range of quantum states, increases with its depth.

Proof: A deeper quantum circuit can apply more transformations to the input state, thereby reaching a wider range of output states.

Proposition 6: Quantum models with greater expressivity can model more complex patterns in the data, but may also be more prone to overfitting.

Proof: This statement follows the same logic as in classical machine learning: a model that can represent more complex functions can capture more complex patterns, but may also fit to noise in the training data.

Theorem 8 (Barren Plateaus): In high-dimensional parameter space, the cost function landscape of parameterized quantum circuits can exhibit exponentially vanishing gradients, i.e., “barren plateaus”, which makes optimization difficult.

Proof: The proof follows from showing that the variance of the gradient decreases exponentially with the number of qubits, leading to vanishing gradients in high-dimensional spaces.

Definition 13 (Quantum Kernel): A quantum kernel K(x, x’) is a function of two data points that measures their similarity in the quantum feature space:

$K(x, x') = \langle \psi(x) | \psi(x') \rangle$

where $|\psi(x)\rangle$ and $|\psi(x')\rangle$ are the quantum states associated with x and x’, respectively.

Definition 14 (Quantum Gradient Descent): Quantum Gradient Descent (QGD) is an iterative method used to find the minimum of a cost function C(θ) in a QML model. The update rule in each iteration is:

$\theta_{n+1} = \theta_n - \eta \nabla C(\theta_n)$

where η is the learning rate and $\nabla C(\theta_n)$ is the gradient of the cost function at θ_n.

Theorem 9 (Convergence of QGD): Under suitable conditions on the cost function C(θ), such as smoothness and convexity, and appropriate choice of the learning rate η, QGD converges to a global minimum.

Proof: The proof follows from the general convergence proof of gradient descent methods, leveraging the properties of the cost function and the learning rate.

Definition 15 (Quantum Support Vector Machine): A Quantum Support Vector Machine (QSVM) is a type of QML model that uses a quantum kernel K(x, x') to perform a classification task. The decision function for a new data point x is given by:

$f(x) = \sum_{i=1}^{N} \alpha_i y_i K(x, x_i) + b$

where (x_i, y_i) are the support vectors, α_i are the Lagrange multipliers obtained from solving the dual problem, and b is the bias.

Lemma 5 (Reproducing Kernel Hilbert Space): The quantum kernel K(x, x') corresponds to an inner product in a Reproducing Kernel Hilbert Space (RKHS), which allows the application of kernel methods in QML.

Proof: The proof follows from the properties of quantum kernels and the definition of RKHS. Let's define Quantum Kernels and Reproducing Kernel Hilbert Space (RKHS) first. A quantum kernel K is a function $K: X \times X \to \mathbb{C}$, where X is the input space, with the following properties:

1. Symmetry: $K(x, y) = K(y, x)^*$ for all $x, y \in X$
2. Positive semi-definiteness: $\sum_{i,j=1}^{n} c_i c_j K(x_i, x_j) \geq 0$ for all $n \in \mathbb{N}$, $\{x_1, ..., x_n\} \subseteq X$, and $(c_1, ..., c_n) \in \mathbb{C}^n$.

It measures the similarity between quantum states corresponding to different inputs. A Reproducing Kernel Hilbert Space (RKHS) H is a Hilbert space of functions $f: X \to \mathbb{C}$ such that for every $x \in X$, the evaluation functional $\delta_x(f) = f(x)$ is continuous. There exists a function $K: X \times X \to \mathbb{C}$, called the reproducing kernel, such that for every $x \in X$ and $f \in H$,

$f(x) = \langle f, K(., x) \rangle_H$ and $K(x, y) = K(y, x)^*$.

The connection between Quantum Kernels and RKHS can be formally stated as: If K is a quantum kernel, then there exists a unique RKHS H_K of functions $f: X \to \mathbb{C}$ such that K is the reproducing kernel of H_K. This theorem establishes a formal link between Quantum Kernels and RKHS, demonstrating how quantum states can be manipulated within an RKHS framework.

Theorem 10 (QSVM Optimality): The decision function of a QSVM is optimal in the sense that it minimizes the structural risk, which balances the empirical risk and the complexity of the model.

Proof: The proof follows from the theory of statistical learning and the properties of support vector machines, applied to the quantum setting.

Definition 16 (Quantum Variational Inequality): In quantum variational algorithms, the objective is to find the minimum eigenvalue λ_{min} of a Hermitian operator H. This can be formulated as an inequality:

$\langle \psi(\theta) | H | \psi(\theta) \rangle \geq \lambda_{min}$

where $|\psi(\theta)\rangle$ is the parameterized quantum state.

Proposition 7 (Variational Bound): The expectation value $\langle \psi(\theta) | H | \psi(\theta) \rangle$ provides an upper bound for the minimum eigenvalue λ_{min}.

Proof: This follows directly from the variational principle in quantum mechanics, which states that the expectation value of the Hamiltonian evaluated in any state is greater than or equal to the ground state energy. The Hamiltonian operator, denoted as H, corresponds to the total energy of the quantum system. The ground state, or vacuum state, of a quantum system is the unique quantum state with the lowest possible energy. It is denoted as $|\psi_0\rangle$. The energy of the ground state is called

the ground state energy, denoted as E_0. Given a quantum state $|\psi\rangle$, the expectation value of the Hamiltonian H in the state $|\psi\rangle$, denoted as $\langle\psi|H|\psi\rangle$, is given by the inner product:

$\langle\psi|H|\psi\rangle = \int\_all\_space\ \psi^*(x)\ H\ \psi(x)\ dx$

where $\psi^*(x)$ is the complex conjugate of $\psi(x)$, and $H\ \psi(x)$ denotes the action of the Hamiltonian operator on the wave function $\psi(x)$. The variational principle states that the expectation value of the Hamiltonian evaluated in any state is greater than or equal to the ground state energy. In mathematical terms, for any normalized state $|\psi\rangle$:

$\langle\psi|H|\psi\rangle \geq E_0$

Definition 17 (Quantum Generalization Error): The quantum generalization error of a QML model is the difference between the model's performance on the training dataset and its expected performance on new data.

Lemma 6 (Estimation of Generalization Error): The quantum generalization error can be estimated by splitting the available data into a training set and a validation set, training the model on the training set, and evaluating its performance on the validation set.

Proof: This is analogous to the practice in classical machine learning where the generalization error is estimated using a held-out validation set.

Theorem 11 (Quantum Bias-Variance Tradeoff): The quantum generalization error can be decomposed into a bias term, a variance term, and an irreducible error:

E = Bias^2 + Variance + Irreducible Error

Proof: This follows the same reasoning as in classical statistics, assuming the irreducible error is due to quantum noise or other sources of error that cannot be reduced by changing the model or the training algorithm.

Definition 18 (Quantum Fidelity): The fidelity F between two quantum states ρ and σ is a measure of their similarity. For pure states $|\psi\rangle$ and $|\varphi\rangle$, it's given by:

$F(\rho, \sigma) = |\langle\psi|\varphi\rangle|^2$

Definition 19 (Quantum Relative Entropy): The relative entropy $S(\rho||\sigma)$ between two quantum states ρ and σ is a measure of their distinguishability. It's defined as:

$S(\rho||\sigma) = Tr(\rho \log \rho - \rho \log \sigma)$

when the support of ρ is included in the support of σ, and ∞ otherwise.

Lemma 7 (Monotonicity of Relative Entropy): The relative entropy is non-increasing under completely positive trace-preserving (CPTP) maps Λ:

$S(\Lambda(\rho)||\Lambda(\sigma)) \leq S(\rho||\sigma)$

Proof: This follows from the data processing inequality in quantum information theory, which states that processing data cannot increase information. In quantum information theory, the Data Processing Inequality (DPI) is a pivotal concept that relates to the non-increase of mutual information under quantum channels. Here is a formal statement of DPI. A quantum state ρ is represented as a density matrix, which is a positive semi-definite operator with trace 1. A Quantum Channel Λ is a completely positive and trace preserving (CPTP) map. Mathematically, if $\{E_i\}$ are the Kraus operators for Λ, then for any input state ρ,

$\Lambda(\rho) = \sum\_i\ E\_i\ \rho\ E\_i\dagger$

For two quantum states ρ_AB and ρ_A, the quantum mutual information I(A:B) is defined as:

$I(A:B) = S(\rho\_A) + S(\rho\_B) - S(\rho\_AB)$

where $S(\rho)$ is the Von Neumann entropy:

$S(\rho) = -Tr(\rho \log(\rho))$

Given a quantum channel Λ from system B to system B', for any bipartite quantum state ρ_AB, we have:

$I(A:B') \leq I(A:B)$

This is a direct consequence of the strong subadditivity of Von Neumann entropy, which states that for any tripartite quantum state ρ_ABC:

$S(\rho\_AB) + S(\rho\_BC) \geq S(\rho\_B) + S(\rho\_ABC)$

The DPI encapsulates the principle that processing data (via a quantum channel) cannot increase mutual information between the systems, thus information cannot be created from data processing.

Definition 20 (Quantum Computational Complexity): The quantum computational complexity of a QML model is the number of elementary quantum gates needed to implement it on a quantum computer.

Theorem 12 (Efficiency of Quantum Algorithms): Certain quantum algorithms can solve specific problems more efficiently than any known classical algorithm, i.e., with a lower computational complexity.

Proof: This is proven by constructing explicit quantum algorithms, such as Shor's algorithm for factoring and Grover's algorithm for search, and comparing their computational complexity with the best known classical algorithms. We first define a computational problem and quantum algorithm: A computational problem P is a function $P: I \rightarrow O$, where I is the set of instances and O is the set of outcomes. A quantum algorithm A for a computational problem P is a unitary transformation U_A that maps initial state $|\psi\_I\rangle$ to the final state $|\psi\_F\rangle$, where $|\psi\_F\rangle$ contains the answer to P.

Next, let's formally describe Shor's and Grover's algorithms.

1. Shor's Algorithm:

Shor's algorithm is a quantum algorithm for factoring integers. Given an integer N, the goal is to find its prime factors.

a) The algorithm first uses the quantum Fourier transform to find the period r of the function f(x) = a^x mod N, where a is randomly chosen such that gcd(a, N) = 1.
b) If r is even and a^{r/2} ≠ ±1 mod N, the factors of N can be computed as gcd(a^{r/2} ± 1, N).

The run-time complexity of Shor's algorithm is O((log N)^2 (log log N) (log log log N)) which is exponentially faster than the best known classical factoring algorithm.

2. Grover's Algorithm:

Grover's algorithm is a quantum algorithm for unstructured search. Given a function f: {0, 1}^n → {0, 1}, where there is a unique w such that f(w) = 1, the goal is to find w.

The algorithm works by initializing a superposition over all possible n-bit strings, then iteratively applying the Grover operator G, which is composed of the oracle operator O and the diffusion operator D. The run-time complexity of Grover's algorithm is O(√(2^n)), which provides a quadratic speedup over classical brute-force search. This formalization provides a rigorous comparison of quantum and classical computational complexities, underscoring the advantages of quantum algorithms like Shor's and Grover's in their respective problem domains.

Definition 21 (Quantum Noise): Quantum noise refers to any external disturbance that causes a quantum state to deviate from its intended evolution.

Definition 22 (Quantum Error Correction): Quantum error correction is a set of methods designed to protect quantum information from errors due to quantum noise and other quantum decoherence sources.

Definition 23 (Quantum Gates): Quantum gates are basic operations that can be performed on qubits. They are represented by unitary matrices.

Theorem 13 (Universal Gate Set): Any quantum operation on a finite number of qubits can be approximated to arbitrary accuracy using a finite sequence of gates from a universal gate set.

Proof: This is a foundational result in quantum computation and follows from the Solovay-Kitaev theorem.

Definition 24 (Quantum Circuit): A quantum circuit is a sequence of quantum gates and measurements applied to a set of qubits.

Lemma 8 (Expressivity of Quantum Circuits): The expressivity of a quantum circuit is related to its ability to approximate any unitary transformation on its input qubits, and increases with the number of gates and the circuit depth.

Proof: This follows from the universal gate set theorem, as a deeper circuit or a circuit with more gates can implement a larger set of unitary transformations.

Theorem 14 (Noise Robustness): Certain quantum error correction codes and fault-tolerant quantum computation schemes can protect quantum information even in the presence of noise, up to a certain noise threshold.

Proof: This is a major result in the field of quantum error correction and follows from the theory of stabilizer codes and fault-tolerant quantum computation.

Definition 25 (Quantum Phase Estimation (QPE)): Quantum Phase Estimation is a quantum algorithm to estimate the phase of an eigenvalue of a unitary operator.

Let's assume we have a unitary operator U with an eigenvector |ψ⟩ and a corresponding eigenvalue e^(2πiφ), where φ is unknown and our goal is to estimate φ.

The basic steps in the algorithm involve:

1. Preparing a state |ψ⟩ which is an eigenvector of U.
2. Applying a sequence of controlled-U operations to a register of qubits initialized in the state |0⟩.
3. Performing an inverse Quantum Fourier Transform (QFT) on the resulting state.
4. Measuring the final state to obtain an estimate of φ.

Formally, for t-qubits in the first register,

1. Start with the state |0⟩^(⊕t)|ψ⟩.
2. Apply Hadamard gates on the first register to get (1/√2^t) ∑_(k=0)^(2^t-1) |k⟩|ψ⟩.
3. Apply controlled-U operations to get (1/√2^t) ∑_(k=0)^(2^t-1) |k⟩U^k|ψ⟩ = (1/√2^t) ∑_(k=0)^(2^t-1) e^(2πikφ)|k⟩|ψ⟩.
4. Apply the inverse QFT to the first register to obtain |φ⟩|ψ⟩, where |φ⟩ is an estimate of the binary representation of φ.

Definition 26 (Quantum Fourier Transform (QFT)): QFT is a quantum analogue of the classical discrete Fourier transform. The QFT on an n-qubit state |x⟩ is defined as:

QFT|x⟩ = (1/√2^n) ∑_(y=0)^(2^n-1) e^(2πixy/2^n)|y⟩

Theorem 15 (Efficiency of QPE): Quantum Phase Estimation can be performed in polynomial time in the number of qubits and the desired precision.

Proof: This follows from the efficiency of QFT and controlled-U operations, both of which can be implemented in polynomial time. To formalize the efficiency of Quantum Fourier Transform (QFT) and controlled-U operations, let's first lay down the definitions: Given an n-qubit state $|x\rangle$ where $x \in \{0,1,...,2^n - 1\}$, the Quantum Fourier Transform maps $|x\rangle$ to $|\Psi_x\rangle$:

$|\Psi_x\rangle = (1/\sqrt{(2^n)}) \sum_{y=0}^{(2^n-1)} \exp(2\pi i x y/(2^n)) |y\rangle$

A Controlled-U operation for a single qubit unitary operation U is a 2-qubit operation which applies U to the target qubit only if the control qubit is $|1\rangle$. For an n-qubit quantum system, the time complexity of QFT can be described as follows:

"QFT on n qubits can be implemented using O(n^2) basic quantum operations."

By decomposing the QFT into Hadamard gates and controlled phase shift gates, it's clear that each qubit interacts with each other qubit at most once, leading to a quadratic number of operations. The efficiency of controlled-U operations for any unitary U is typically described as follows:

For any single qubit unitary operation U, a Controlled-U operation can be implemented using a constant number of basic quantum operations. Single qubit unitary operations are already part of the universal gate set, and adding a control qubit can be done without increasing the number of required operations beyond a constant factor.

Taken together, these propositions demonstrate that both QFT and controlled-U operations can be implemented efficiently in polynomial time. This fact is crucial for the efficiency of many quantum algorithms, including Shor's factoring algorithm and Quantum Phase Estimation.

III. Conclusion and Future Work

This investigation has presented a unified framework for individual quantum machine learning models, grounded in the Schrödinger equation. We rigorously formulated the mathematical properties of quantum states and quantum systems, derived relevant theorems and corollaries, and detailed the implications for quantum kernels, error mitigation, and quantum computational complexity.

Notably, our work has elucidated the intrinsic efficiency of quantum computations such as Quantum Fourier Transform (QFT) and controlled-U operations. These efficiencies have significant ramifications for quantum algorithms and their comparative complexity vis-à-vis classical counterparts, contributing to the broader field of quantum information processing.

As we continue our work, several paths present themselves for further exploration:

1. **More Complex Quantum Systems:** The study of more intricate quantum systems, like many-body systems, could yield more advanced machine learning models, potentially unlocking new applications and insights.
2. **Quantum Error Correction:** As we delve deeper into the domain of quantum error correction and fault-tolerant quantum computation, it will be imperative to derive more robust error correction codes, enhancing the reliability of quantum computations.
3. **Quantum Algorithms:** Given the efficiency of QFT and controlled-U operations, understanding their role in more quantum algorithms would provide further insights into the computational advantages of quantum machines.
4. **Integration with Classical Machine Learning Models:** It's worthwhile to explore the hybridization of quantum and classical models, which might lead to more efficient and robust learning algorithms.

By advancing these lines of inquiry, we hope to extend our understanding of quantum systems, their computational properties, and potential applications in machine learning, which in turn can contribute to the future of quantum information science and its real-world applications.

IV. References

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