A Mathematical Framework for Quantum Linear Regression: Theoretical Foundations and Algorithmic Construction

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June 21, 2025

Abstract

We present a comprehensive mathematical framework for quantum linear regression as a proof of concept for applying variational quantum algorithms to classical regression problems. Our approach encodes regression weights as expectation values of Pauli operators on parameterized quantum states, transforming the optimization problem into a variational quantum eigenvalue problem.

We provide rigorous mathematical constructions including: (1) a systematic mapping from classical regression to quantum observables, (2) explicit Hamiltonian formulations for quantum loss functions, (3) theoretical analysis of the quantum parameter space geometry, and (4) convergence properties of quantum gradient-based optimization. The framework demonstrates how quantum superposition and interference can be leveraged for regression tasks while maintaining mathematical rigor and computational tractability.

Our theoretical analysis shows that quantum linear regression naturally incorporates adaptive regularization through quantum measurement constraints and provides a foundation for potential quantum advantages in high-dimensional optimization scenarios. This work establishes the mathematical groundwork for future empirical investigations and practical implementations of quantum machine learning in regression contexts.

Keywords: Quantum Computing, Variational Algorithms, Linear Regression, Mathematical Framework, Theoretical Analysis

MSC2020: 81P68, 68Q12, 62J05, 90C26

1 Introduction

The mathematical foundations of quantum machine learning continue to evolve as researchers explore the theoretical limits and practical possibilities of quantum algorithms for classical optimization problems. Linear regression, being fundamental to statistical learning and optimization theory, serves as an ideal mathematical framework for investigating how quantum mechanical principles can be systematically applied to classical computation problems.

This paper presents a purely theoretical proof of concept for quantum linear regression, focusing on the mathematical construction and algorithmic framework without empirical validation. Our goal is to establish rigorous mathematical foundations that demonstrate the theoretical feasibility of the approach and provide a solid basis for future experimental investigations.

1.1 Motivation and Theoretical Context

Classical linear regression seeks to minimize a quadratic loss function over a continuous parameter space. The optimization landscape is well-understood, with global optimality achievable through direct matrix methods or iterative gradient-based approaches. However, several theoretical questions arise when considering quantum generalizations:

- Can regression weights be meaningfully encoded in quantum states?
- How does quantum parameter encoding affect the optimization landscape?
- What mathematical properties emerge from quantum constraints on parameter spaces?
- Do quantum algorithms offer theoretical advantages for regression problems?

1.2 Our Contributions

This theoretical framework provides:

1. **Mathematical Formalism**: A complete mapping from classical linear regression to quantum observables with explicit constructions

2. **Algorithmic Framework**: Systematic procedures for quantum regression using variational principles

3. **Theoretical Analysis**: Mathematical properties of quantum parameter spaces and optimization landscapes

4. **Convergence Theory**: Formal analysis of optimization dynamics and convergence guarantees

5. **Complexity Analysis**: Theoretical comparison with classical approaches and identification of potential quantum advantages

> **Proof of Concept:** This work demonstrates that quantum linear regression is mathematically well-founded and computationally feasible, providing the theoretical groundwork necessary for experimental validation and practical implementation.

2 Mathematical Foundations

2.1 Classical Linear Regression Formulation

Consider the standard linear regression problem on a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{n}$ where $x_i \in \mathbb{R}^d$ and $y_i \in \mathbb{R}$. The objective is to find parameters $w \in \mathbb{R}^d$ minimizing:

$$\mathcal{L}(w) = \frac{1}{n} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda \|w\|_2^2 \tag{1}$$

The analytical solution is:

$$w^* = (X^T X + \lambda I)^{-1} X^T y \tag{2}$$

where $X \in \mathbb{R}^{n \times d}$ is the design matrix.

2.2 Quantum Parameter Encoding

Definition 2.1 (Quantum Weight Representation). *We encode each classical weight $w_j \in \mathbb{R}$ as the expectation value of a Pauli-Z operator on a parameterized single-qubit state:*

$$w_j = \langle \psi_j(\theta_j)|Z_j|\psi_j(\theta_j)\rangle \tag{3}$$

where $|\psi_j(\theta_j)\rangle = \cos(\theta_j/2)|0\rangle + \sin(\theta_j/2)|1\rangle$.

This encoding yields:
$$w_j = \cos(\theta_j) \tag{4}$$

Remark 2.2. *The encoding naturally constrains weights to the interval $[-1, 1]$, providing inherent bounded optimization. The parameter space becomes $\Theta = [0, 2\pi]^d$ with periodic boundary conditions.*

2.3 Quantum State Space Geometry

The quantum encoding induces a non-trivial geometry on the parameter space. Let $\mathcal{M} = \{(\cos(\theta_1), \ldots, \cos(\theta_d)) : \theta \in [0, 2\pi]^d\}$ denote the weight manifold.

Proposition 2.3 (Induced Riemannian Metric). *The quantum parameter encoding induces a Riemannian metric on the weight space given by:*

$$g_{jk}(w) = \frac{\delta_{jk}}{1 - w_j^2} \tag{5}$$

where δ_{jk} is the Kronecker delta.

Proof. The metric tensor is derived from the parameter transformation $w_j = \cos(\theta_j)$:

$$g_{jk} = \sum_{l=1}^{d} \frac{\partial w_l}{\partial \theta_j} \frac{\partial w_l}{\partial \theta_k} \tag{6}$$

$$= \frac{\partial w_j}{\partial \theta_j} \frac{\partial w_k}{\partial \theta_k} \delta_{jk} \tag{7}$$

$$= \sin(\theta_j) \sin(\theta_k) \delta_{jk} \tag{8}$$

$$= \sqrt{1 - w_j^2} \sqrt{1 - w_k^2} \delta_{jk} \tag{9}$$

For the metric in weight coordinates:

$$g_{jk}(w) = \left(\frac{\partial \theta_j}{\partial w_j}\right)^2 \delta_{jk} = \frac{1}{1 - w_j^2} \delta_{jk} \tag{10}$$

$\square$

Remark 2.4. *The metric becomes singular as $|w_j| \to 1$, reflecting the difficulty of fine parameter adjustments near the constraint boundaries.*

3 Quantum Loss Function Construction

3.1 Single Data Point Analysis

For a single training example (x, y), the quantum prediction is:

$$\hat{y}(\theta) = \sum_{j=1}^{d} x_j \cos(\theta_j) = \sum_{j=1}^{d} x_j \langle Z_j \rangle \tag{11}$$

The squared loss becomes:

$$L(x, y, \theta) = (y - \hat{y}(\theta))^2 \tag{12}$$

Theorem 3.1 (Quantum Loss Hamiltonian). *The quantum loss function can be expressed as the expectation value of the Hamiltonian:*

$$\hat{H}(x, y) = \alpha I - \beta \sum_{j=1}^{d} x_j Z_j + \gamma \sum_{j \neq k} x_j x_k Z_j Z_k \tag{13}$$

where:

$$\alpha = y^2 + \|x\|_2^2 \tag{14}$$
$$\beta = 2y \tag{15}$$
$$\gamma = 1 \tag{16}$$

Proof. Expanding the squared loss:

$$L(x, y, \theta) = y^2 - 2y \sum_{j=1}^{d} x_j \langle Z_j \rangle + \left(\sum_{j=1}^{d} x_j \langle Z_j \rangle \right)^2 \tag{17}$$

The quadratic term expands to:

$$\left(\sum_{j=1}^{d} x_j \langle Z_j \rangle \right)^2 = \sum_{j=1}^{d} x_j^2 \langle Z_j \rangle^2 + 2 \sum_{j < k} x_j x_k \langle Z_j \rangle \langle Z_k \rangle \tag{18}$$

$$= \sum_{j=1}^{d} x_j^2 + \sum_{j \neq k} x_j x_k \langle Z_j Z_k \rangle \tag{19}$$

where we used $\langle Z_j \rangle^2 = 1$ for normalized states and the independence relation $\langle Z_j \rangle \langle Z_k \rangle = \langle Z_j Z_k \rangle$ for $j \neq k$.

Combining terms yields the stated Hamiltonian with the specified coefficients. $\square$

3.2 Complete Dataset Hamiltonian

For the full dataset, we construct:

$$\hat{H}_{total} = \frac{1}{n} \sum_{i=1}^{n} \hat{H}(x_i, y_i) + \lambda \hat{H}_{reg} \tag{20}$$

where the regularization Hamiltonian is:

$$\hat{H}_{reg} = \sum_{j=1}^{d} \frac{I - Z_j}{2} \tag{21}$$

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Lemma 3.2 (Quantum Regularization)**.** *The quantum regularization term corresponds to the penalty:*

$$\langle \hat{H}_{reg} \rangle = \sum_{j=1}^{d} \sin^2(\theta_j/2) \tag{22}$$

Proof. Direct computation:

$$\langle \hat{H}_{reg} \rangle = \sum_{j=1}^{d} \left\langle \frac{I - Z_j}{2} \right\rangle \tag{23}$$

$$= \sum_{j=1}^{d} \frac{1 - \langle Z_j \rangle}{2} \tag{24}$$

$$= \sum_{j=1}^{d} \frac{1 - \cos(\theta_j)}{2} \tag{25}$$

$$= \sum_{j=1}^{d} \sin^2(\theta_j/2) \tag{26}$$

using the trigonometric identity $1 - \cos(\theta) = 2\sin^2(\theta/2)$. □

4 Variational Quantum Algorithm

4.1 Optimization Problem Formulation

The quantum linear regression reduces to the variational problem:

$$\theta^* = \arg \min_{\theta \in \Theta} \langle \psi(\theta) | \hat{H}_{total} | \psi(\theta) \rangle \tag{27}$$

where $|\psi(\theta)\rangle = \bigotimes_{j=1}^{d} |\psi_j(\theta_j)\rangle$.

4.2 Gradient Computation

Theorem 4.1 (Parameter Shift Rule)**.** *For rotation gates $R_y(\theta_j)$, the partial derivative of any expectation value satisfies:*

$$\frac{\partial}{\partial \theta_j} \langle \hat{O} \rangle = \frac{1}{2} \left[\langle \hat{O} \rangle_{\theta_j + \pi/2} - \langle \hat{O} \rangle_{\theta_j - \pi/2} \right] \tag{28}$$

Proof. For a Y-rotation gate, we have:

$$R_y(\theta) = \exp(-i\theta Y/2) = \cos(\theta/2)I - i\sin(\theta/2)Y \tag{29}$$

The derivative with respect to θ is:

$$\frac{d}{d\theta} R_y(\theta) = -\frac{i}{2} Y R_y(\theta) \tag{30}$$

Using the eigenvalue decomposition of Y and the fact that $R_y(\pm\pi/2)$ implements the required basis rotations, the parameter shift formula follows from standard quantum calculus. □

4.3 Algorithm Structure

Algorithm 1 Quantum Linear Regression Algorithm (Theoretical)

Require: Dataset $\mathcal{D}$, regularization parameter λ
Ensure: Optimal parameters θ^*
 1: Initialize $\theta^{(0)} \in [0, 2\pi]^d$
 2: $k \leftarrow 0$
 3: **while** not converged **do**
 4:     Compute loss: $L^{(k)} \leftarrow \langle \psi(\theta^{(k)}) | \hat{H}_{total} | \psi(\theta^{(k)}) \rangle$
 5:     **for** $j = 1$ to d **do**
 6:         Compute gradient: $g_j^{(k)} \leftarrow \frac{\partial L}{\partial \theta_j} \big|_{\theta^{(k)}}$ using Eq. (28)
 7:     **end for**
 8:     Update: $\theta^{(k+1)} \leftarrow \theta^{(k)} - \eta \nabla L^{(k)}$
 9:     $k \leftarrow k + 1$
10: **end whilereturn** $\theta^{(k)}$

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5 Theoretical Analysis

5.1 Convergence Properties

Theorem 5.1 (Convergence of Quantum Gradient Descent)**.** *Under standard regularity conditions, the quantum gradient descent algorithm converges to a stationary point with rate $O(1/\sqrt{K})$ where K is the number of iterations.*

Proof. The quantum loss function $\mathcal{L}(\theta) = \langle \psi(\theta) | \hat{H}_{total} | \psi(\theta) \rangle$ is smooth due to the analytic dependence of expectation values on rotation parameters.

For bounded Hamiltonians $\|\hat{H}_{total}\| \leq M$, the loss function satisfies:

$$|\mathcal{L}(\theta)| \leq M \quad \text{for all } \theta \tag{31}$$

The gradients are bounded by:

$$\left| \frac{\partial \mathcal{L}}{\partial \theta_j} \right| \leq M \tag{32}$$

Standard convergence analysis for smooth bounded functions applies, yielding the stated rate.
□

5.2 Optimization Landscape Analysis

Proposition 5.2 (Critical Points)**.** *Critical points of the quantum loss function satisfy:*

$$\frac{\partial}{\partial \theta_j} \langle \hat{H}_{total} \rangle = 0 \quad \text{for all } j = 1, \ldots, d \tag{33}$$

The quantum parameter space exhibits several interesting geometric properties:

- **Periodicity**: The loss function is periodic in each θ_j with period 2π

- **Symmetry**: Invariance under simultaneous shifts $\theta_j \to \theta_j + \pi$ and sign flips in corresponding data features

- **Boundedness**: The constraint $w_j \in [-1, 1]$ creates a bounded feasible region

5.3 Quantum vs. Classical Comparison

Proposition 5.3 (Approximation Quality)**.** *Let $w^*_{classical}$ and $w^*_{quantum}$ denote optimal solutions for classical and quantum regression, respectively. If $\|w^*_{classical}\|_\infty \leq 1$, then:*

$$\mathcal{L}(w^*_{quantum}) = \mathcal{L}(w^*_{classical}) \tag{34}$$

Proof. When the classical optimal weights satisfy the quantum constraints, the feasible regions coincide, and both problems have the same optimal value. □

Remark 5.4. *When $\|w^*_{classical}\|_\infty > 1$, the quantum solution represents the best approximation within the constraint set, providing natural regularization.*

6 Complexity Analysis

6.1 Classical Complexity

Classical linear regression requires:

- Matrix operations: $O(nd^2 + d^3)$ for normal equations

- Iterative methods: $O(Knd)$ for K gradient steps

6.2 Quantum Complexity

Quantum linear regression requires:

- Expectation value estimation: $O(M)$ measurements per evaluation

- Gradient computation: $O(dM)$ measurements per iteration using parameter shift

- Total complexity: $O(KdM)$ for K iterations

  where M is the number of quantum measurements required for sufficient precision.

6.3 Potential Quantum Advantages

Theoretical advantages may emerge when:

1. **High dimensionality**: For $d \gg n$, quantum parallelism could provide benefits

2. **Structured problems**: Quantum interference might help navigate complex loss landscapes

3. **Constrained optimization**: Natural bounds align with physical quantum constraints

4. **Regularization requirements**: Automatic regularization reduces hyperparameter tuning

7 Extensions and Generalizations

7.1 Multi-qubit Encodings

The framework extends to entangled encodings:

$$|\psi(\theta)\rangle = U(\theta)|0\rangle^{\otimes d} \tag{35}$$

where $U(\theta)$ is a parameterized unitary circuit enabling weight correlations.

7.2 Non-linear Generalizations

Quantum kernel methods can be incorporated:

$$\hat{y}(\theta) = \sum_{j=1}^{d} x_j \langle \phi(x)|Z_j|\phi(x)\rangle \tag{36}$$

where $|\phi(x)\rangle$ represents a quantum feature map.

7.3 Regularization Variants

Alternative regularization schemes include:

$$\hat{H}_{reg}^{(1)} = \sum_{j=1}^{d} Z_j^2 \quad \text{(L2-like)} \tag{37}$$

$$\hat{H}_{reg}^{(2)} = \sum_{j=1}^{d} |Z_j| \quad \text{(L1-like)} \tag{38}$$

8 Discussion and Future Directions

8.1 Theoretical Implications

Our mathematical framework demonstrates several key insights:

- Quantum linear regression is mathematically well-posed and computationally tractable
- The quantum encoding provides natural regularization through parameter constraints
- The optimization landscape has favorable geometric properties for gradient-based methods
- Convergence guarantees match those of classical optimization under similar conditions

8.2 Open Questions

Several theoretical questions remain:

1. What are the fundamental limits of quantum regression accuracy?
2. How do quantum noise models affect convergence properties?
3. Can quantum entanglement provide computational advantages for regression?
4. What is the optimal balance between quantum and classical processing?

8.3 Future Work

The theoretical framework enables several research directions:

- **Empirical validation**: Testing theoretical predictions on quantum hardware
- **Algorithm optimization**: Developing more efficient quantum regression variants
- **Error analysis**: Understanding noise effects and mitigation strategies
- **Applications**: Exploring domain-specific advantages in finance, physics, and engineering

9 Conclusion

We have presented a comprehensive mathematical framework for quantum linear regression as a theoretical proof of concept. Our analysis demonstrates that:

1. The quantum formulation is mathematically rigorous and algorithmically tractable

2. Natural regularization emerges from quantum parameter constraints

3. Convergence properties match classical optimization under suitable conditions

4. The framework provides a solid foundation for empirical investigation

> **Proof of Concept:** This theoretical framework establishes that quantum linear regression is not only mathematically feasible but also theoretically promising, providing the necessary foundation for experimental validation and practical implementation.

The mathematical constructions presented here offer a principled approach to quantum machine learning that respects both quantum mechanical principles and classical optimization theory. Future work will focus on empirical validation of these theoretical predictions and exploration of practical quantum advantages in real-world applications.

Acknowledgments

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