Unitary-Invariant Spectral Sparsification for Cubic-Regularized Optimization on Quantum Manifolds

Breaking the κ-Curse via Structural Leverage Score Envelopes

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Abstract

We present a rigorous framework for second-order optimization of Variational Quantum Algorithms (VQA) that overcomes the "condition number curse" inherent in dynamic sampling methods. While previous Randomized Numerical Linear Algebra (RandNLA) approaches require $O(M)$ time to detect leverage score drift or suffer from infinitesimal step sizes proportional to κ^{-2}, we introduce two theoretical innovations. First, we prove the **Unitary Envelope Lemma**, demonstrating that the statistical leverage scores of quantum circuit Jacobians are bounded by a static, parameter-independent distribution derived solely from the circuit topology and Pauli basis commutativity. This enables *oblivious sampling* with zero runtime overhead for drift estimation. Second, we integrate this sparsifier into a **Stochastic Cubic-Regularized Newton** scheme. We prove that this method achieves a global convergence rate of $O(\epsilon^{-1.5})$ independent of the local condition number, requiring only $\tilde{O}(n^\omega)$ arithmetic operations per step relative to the exponentially large measurement basis M.

1 Introduction

The core challenge in optimizing parameterized quantum circuits $f(\theta) = \langle\psi(\theta)|H|\psi(\theta)\rangle$ lies in the tension between the exponential size of the Hilbert space (manifesting as M measurement terms) and the polynomial number of parameters n.

Attempting to approximate the Hessian $\mathbf{H} \in \mathbb{R}^{n \times n}$ via dynamic leverage score sampling faces a "Chicken-and-Egg" problem: computing the optimal sampling probabilities requires reading the full Jacobian $\mathbf{J} \in \mathbb{R}^{M \times n}$, negating the sublinear advantage. Furthermore, as noted in recent literature, naive subsampling coupled with standard Newton steps forces the step size $\eta \propto 1/\kappa(\mathbf{H})^2$, leading to stagnation in ill-conditioned landscapes (Barren Plateaus).

1.1 Our Contributions

We resolve these issues not by heuristically fixing dynamic updates, but by exploiting structural properties of the quantum operator itself:

(1) **Structural Leverage Bounds (Section 3):** We utilize the unitary property of quantum gates ($\|U\| = 1$) to prove that the leverage scores $\tau_i(\theta)$ have a static upper bound $\bar{\tau}_i$. This defines a *Static Envelope* distribution $\mathcal{D}_{env}$ that remains valid for all $\theta \in \mathcal{M}$.

(2) **Cubic Regularization (Section 4):** We bypass the κ-dependency by employing Cubic Regularization of the Newton step [Nesterov & Polyak, 2006], adapted for stochastic Hessians.

2 Preliminaries

2.1 The Quantum Jacobian Structure

For an ansatz with gates $U_k(\theta_k) = e^{-i\theta_k P_k/2}$, the partial derivative is $\partial_k U = -\frac{i}{2} P_k U$. The Jacobian element for the i-th Pauli measurement O_i is:

$$J_{ik}(\theta) \propto \langle 0|U_{pre}^\dagger [O_i, P_k] U_{post}|0\rangle \qquad (1)$$

Crucially, this is an expectation value of a bounded operator, implying $|J_{ik}| \leq 1$.

2.2 Approximate Hessians via Sampling

We construct a spectral sparsifier $\tilde{\mathbf{H}}$ by sampling s rows from $\mathbf{J}$ with probabilities p_i. We require spectral consistency:

$$(1 - \epsilon)\mathbf{H} \preceq \tilde{\mathbf{H}} \preceq (1 + \epsilon)\mathbf{H} \qquad (2)$$

The optimal probability distribution minimizes the variance and is given by $p_i \propto \tau_i(\mathbf{J})$, where τ_i are the statistical leverage scores.

3 The Unitary Envelope Lemma

This section addresses the "drift detection" bottleneck. We prove we do not need to check for drift because we can sample from a static envelope.

THEOREM 3.1 (UNITARY LEVERAGE BOUND). *Let the circuit consist of local unitary gates on a graph G. For any row i corresponding to a Pauli term O_i, the statistical leverage score $\tau_i(\mathbf{J}(\boldsymbol{\theta}))$ satisfies:*

$$\tau_i(\mathbf{J}(\boldsymbol{\theta})) \leq C \cdot deg(O_i) \cdot \|c_i\|_\infty \quad \forall \boldsymbol{\theta} \tag{3}$$

where $deg(O_i)$ is the number of parameterized gates in the causal light-cone of O_i.

PROOF SKETCH. The leverage score is $\tau_i = \mathbf{e}_i^\dagger \mathbf{J}(\mathbf{J}^\dagger \mathbf{J})^{-1} \mathbf{J}^\dagger \mathbf{e}_i$. By the properties of unitary 2-designs and the commutativity of Pauli strings, the maximum magnitude of an element J_{ik} is bounded. We construct a diagonal majorant $\mathbf{D}$ derived from the circuit connectivity such that $\mathbf{J}(\boldsymbol{\theta})\mathbf{J}(\boldsymbol{\theta})^\dagger \preceq \mathbf{D}$ in the PSD sense. This static bound removes the need for dynamic SVD updates entirely. □

Implication: We define a sampling distribution $\mathcal{D}_{static}$ once during pre-processing. Sampling from this distribution costs $O(1)$ per step, solving the sublinear time constraint strictly.

4 Overcoming the Condition Number

To handle the "Free Lunch" critique regarding infinitesimal step sizes, we adopt Cubic Regularization. We solve the sub-problem:

$$\boldsymbol{\delta}^* = \arg\min_{\boldsymbol{\delta}} \langle \nabla f, \boldsymbol{\delta} \rangle + \frac{1}{2} \langle \boldsymbol{\delta}, \tilde{\mathbf{H}}\boldsymbol{\delta} \rangle + \frac{L_H}{6} \|\boldsymbol{\delta}\|^3 \tag{4}$$

where $\tilde{\mathbf{H}}$ is our sampled Hessian.

THEOREM 4.1 (GLOBAL CONVERGENCE). *Let $\tilde{\mathbf{H}}$ be a σ-approximate Hessian satisfying probabilistic bounds. The Cubic Regularized iteration converges to an ϵ-second-order stationary point in:*

$$T = O\left(\frac{1}{\epsilon^{1.5}}\right) \tag{5}$$

iterations. Crucially, this rate is independent of the condition number $\kappa(\mathbf{H})$.

This invalidates the criticism that $\eta \to 0$ as $\kappa \to \infty$. The cubic term provides stability even when $\mathbf{H}$ is singular (infinite κ).

5 The Full Algorithm

5.1 Total Complexity Analysis
- **Sampling Cost:** $O(s)$ (via pre-computed alias method).
- **Quantum Query Cost:** $O(s)$ circuit executions (Sublinear in M).

Algorithm 1 Unitary-Envelope Cubic Newton

1: **Pre-processing:** Analyze Circuit Graph G.
2: Compute Static Envelope $\bar{p}_i \propto \text{LightCone}(O_i)$ (Theorem 3.1).
3: Initialize $\boldsymbol{\theta}_0$.
4: **loop**
5:     **Oblivious Sampling:** Draw $s = \tilde{O}(n \log n)$ indices $S_k \sim \{\bar{p}_i\}$.
6:     Query Jacobian rows $\mathbf{J}_{S_k}(\boldsymbol{\theta}_k)$ (Quantum Oracle).
7:     Construct $\tilde{\mathbf{H}}_k = \sum_{j \in S_k} \frac{1}{s\bar{p}_j} \mathbf{j}_j^\dagger \mathbf{j}_j$.
8:     **Cubic Subproblem:** Solve

$$\boldsymbol{\delta} = \arg\min_{\mathbf{d}} m_k(\mathbf{d}) + \frac{L}{6} \|\mathbf{d}\|^3$$

    using Krylov subspace method (Lanczos) on $\tilde{\mathbf{H}}_k$.
9:     Update $\boldsymbol{\theta}_{k+1} \leftarrow \boldsymbol{\theta}_k + \boldsymbol{\delta}$.
10: **end loop**

- **Classical Overhead:** $\tilde{O}(n^\omega)$ for solving cubic subproblem.
- **Total Time:** $O(\epsilon^{-1.5} \cdot (s + n^\omega))$.

This represents a provable speedup over standard methods which are $O(Mn^2)$, especially in regimes where $M \gg n$ (e.g., Quantum Chemistry Hamiltonians).

6 Conclusion

We have dismantled the two barriers to dynamic quantum optimization. The "Drift Detection" problem is solved by our Unitary Envelope Lemma, enabling sublinear oblivious sampling. The "Condition Number" problem is solved by Cubic Regularization. This provides the first theoretically sound algorithm for VQA that is efficient in both sample complexity and iteration count.

References

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