

Quantum Computing based Algorithms for Sparse Matrix Eigenvalue Problems

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Abstract. Eigenvalue problems are integral to numerous scientific and engineering disciplines, arising in contexts such as Mechanical Engineering, Quantum Mechanics, Civil Engineering, Data Science, and Graph Theory. In Mechanical Engineering, these problems involve solving for vibration modes of structures by analyzing their stiffness and mass matrices. In Quantum Mechanics, eigenvalue problems are central to solving the Schrödinger Equation to determine energy eigenvalues and corresponding wave functions. Civil Engineering applications use eigenvalue analysis for determining buckling loads in columns, dependent on the column's stiffness and load distribution. In Data Science, Principle Component Analysis (PCA) leverages eigenvalues for dimensionality reduction. Stability Analysis in Control Theory requires examining the eigenvalues of a system's state matrix to assess stability. Additionally, Graph Theory uses eigenvalue problems to study network properties through the adjacency or Laplacian matrices, providing insights into graph connectivity and centrality. Notably, Google's PageRank algorithm exemplifies the application of eigenvalue problems in practical systems.

Quantum computing, a burgeoning field, offers potential exponential speedups for specific computational problems. Shor's Algorithm, for example, achieves polynomial time complexity $\mathcal{O}((\log N)^3)$ for integer factorization, compared to the best classical algorithms with complexity $2^{\mathcal{O}((\log N)^{1/3}(\log \log N)^{2/3})}$. Grover's Algorithm provides a quadratic speedup in unstructured search tasks, reducing time complexity to $\mathcal{O}(\sqrt{N})$ compared to classical linear search's $\mathcal{O}(N)$. The HHL algorithm shows promise for solving linear systems of equations more efficiently than classical methods.

This paper focuses on developing quantum algorithms for large-scale, sparse, nonlinear eigenvalue problems frequently encountered in Density Functional Theory (DFT). Existing hybrid quantum-classical algorithms, such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE), are constrained by inefficiencies related to matrix sparsity and computational speed. We investigate quantum subspace methods, analogous to classical Krylov subspace methods, to address these challenges in solving differential equations, such as the heat equation.