A Review of Quantum Principle Component Analysis

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1 Introduction

In this work a technique is introduced that enables the eigenvectors corresponding to the dominant eigenvalues of an unknown state to be found exponentially faster than can be done with current classical methods. This technique, quantum principle component analysis, could play a crucial role in the future by providing a tool which could help in speeding up tasks such as state discrimination, clustering and pattern recognition. Quantum component analysis also provides a method for supervised learning and could be essential to future quantum machine learning technology.

It is often desirable to reveal the key properties of an unknown state but due to measurement collapse to a single eigenstate, very little information is obtained about the original state except with repeated measurement and statistical analysis. To uncover the information contained in an unknown quantum state, quantum principle component analysis utilizes the unknown quantum state to perform self-analysis by taking multiple copies of the state with a density matrix ρ and performing the unitary operation $e^{-i\rho t}$. This process, state self tomography, enables one to find and work with the directions in the data space that have the largest variance.

Quantum principle component analysis is based on the idea that geometric intuition of the

most prevalent features of the space can found from studying the eigenvectors of the data. It is limited in that it deals with flat Euclidean structures and cannot find nonlinear structures on the data.[2] The analysis works best when there is a disparity in the eigenvalue magnitudes with some being large. The dominant eigenvalues represent the principal components of the system which dictate the overall dynamics. When a system is dominated by several large eigenvalues, the projection of the system onto a subspace constructed by the corresponding eigenvectors closely resembles the original system and allows for efficient analysis without having to analyze the entire system, which is computationally expensive.

Conventionally in tomography, the state plays a passive role but in qPCA the quantum state's density matrix functions as a Hamiltonian that generates transformations on other states. The core property of quantum principle component analysis is that it makes use of multiple copies of the quantum system or density matrix to reveal its hidden features.

2 Method

Quantum principle component analysis is a two step process. First, multiple copies of a density matrix ρ are used to perform density matrix exponentiation. Secondly, density matrix exponentiation is used in the quantum phase algorithm to reveal features of the eignevectors and eigenvalues of ρ.

Given n copies of the density matrix ρ, the unitary transformation $e^{-i\rho t}$ can generate transformations on a density matrix σ

$$\mathrm{tr}_P e^{-iS\Delta t}\rho \otimes \sigma e^{iS\Delta t} = (\cos^2 \Delta t)\sigma + (\sin^2 \Delta t)\rho - i \sin \Delta t[\rho, \sigma] \tag{1}$$

$$= \sigma - i\Delta t[\rho, \sigma] + O(\Delta t^2). \tag{2}$$

where tr_P is the partial trace over the first variable and S is the sparse swap operator. Repeatedly applying this transformation leads to $e^{-i\rho n\Delta t}\sigma e^{i\rho n\Delta t}$. Once density matrix expo-

nentiation is obtained it is used to apply the quantum phase algorithm to find the eigenvalues and eigenvectors of an unknown density matrix.

The quantum phase algorithm applies the operator $e^{-i\rho n\Delta t}$ at varying time t to take the state $|\psi\rangle|0\rangle$ to $\sum_i \psi_i|\chi_i\rangle|\widetilde{r}_i\rangle$ where $|\chi_i\rangle$ are the eigenvectors of ρ and $\widetilde{r}_i$ are estimates of the corresponding eigenvalues. This process takes a time-order of $O(\log d)$ and is an exponential speed-up over classical principle component analysis.

Quantum principle component analysis can be utilized in quantum machine learning by enabling state discrimination. We wish to take a state $|\chi\rangle$ and determine whether it belongs in a set $\{|\phi_i\rangle\}$, represented by the density matrix ρ, or $\{|\psi_i\rangle\}$, represented by the density matrix σ. This is equivalent to the procedure in supervised learning tasks in which one wishes to determine which class a particular item belongs to, for example whether a picture is of a dog or a cat. To do this, we make use of matrix exponentiation to decompose the state $|\chi\rangle$ in terms of the eigenvectors and eigenvalues of ρ - σ

$$|\chi\rangle|0\rangle \rightarrow \sum_j \chi_j|\epsilon_j\rangle|x_j\rangle \tag{3}$$

where $|\epsilon_j\rangle$ are the eigenvectors of ρ - σ and x_j are the corresponding eigenvalues. A measurement on the first eigenvalue register is performed and if it returns positive than the state $|\chi\rangle$ is classified to set $\{|\phi_i\rangle\}$ and if it is negative it is assigned to $\{|\psi_i\rangle\}$. The validity of the classification can be determined from the value of the measured eigenvalue. Larger magnitude eigenvalues correspond to higher confidence in the assignment.

3 Context

Quantum principle component analysis fits into the broader context of quantum algorithmic methods as being a first approach method to identify structure within data in machine learning tasks. It performs classification by considering only the most dominant eigenvectors within a space. This work by Lloyd et.al [1] provides a proof of principle that quantum

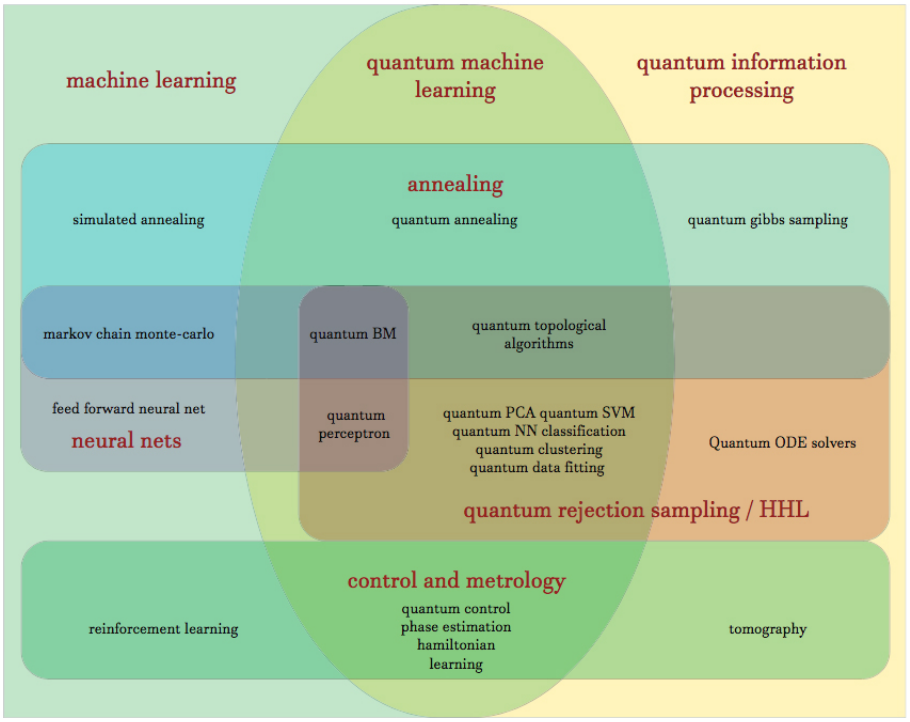

Figure 1: Intersection of Machine Learning and Quantum Computing [3]

computation will be important to the machine learning community and can provide exponential speedup over the correlate classical algorithm. Quantum principle component analysis also can be used in a broader context whenever eigendecomposition is needed for systems characterized by dominant eigenvectors.

Machine learning can be broadly classified into two categories depending upon whether or not it has external help in categorizing the data. In supervised learning, specific examples are given to train the learning system how categorization should be done. This is often done by taking a subset of the available data and having an outside resource provide a label. In unsupervised learning, no external help is given and the learning system must find structure within the data on its own. Various quantum algorithms have been proposed that will provides exponential speed-up over their classical counter-parts. These include quantum principle component analysis, quantum manifold embedding, quantum K-means, quantum K-medians, quantum hierarchical clustering. [2] (See Figure 2)

QPCA is a first step but algorithms that use more complex low dimensional manifolds

Algorithm	Papers	Grover	Speedup	Quantum Data	Gen. Perf.	Implementation
K-medians	Aïmeur et al. (2013)	Yes	Quadratic	No	No	No
Hierarchical clustering	Aïmeur et al. (2013)	Yes	Quadratic	No	No	No
K-means	Lloyd et al. (2013a)	Optional	Exponential	Yes	No	No
Principal components	Lloyd et al. (2013b)	No	Exponential	Yes	No	No
Associative memory	Ventura and Martinez (2000)	Yes		No	No	No
	Trugenberger (2001)	No		No	No	No
Neural networks	Narayanan and Menneer (2000)	Yes		No	Numerical	Yes
Support vector machines	Anguita et al. (2003)	Yes	Quadratic	No	Analytical	No
	Rebentrost et al. (2013)	No	Exponential	Yes	No	No
Nearest neighbors	Wiebe et al. (2014)	Yes	Quadratic	No	Numerical	No
Regression	Bisio et al. (2010)	No		Yes	No	No
Boosting	Neven et al. (2009)	No	Quadratic	No	Analytical	Yes

Figure 2: Quantum machine learning algorithms. [2]

to embed high dimensional information are possible. One such example is the quantum K-means algorithm. This algorithm, based on Grovers search algorithm, calculates centroids and assigns vectors to the closest centroids.[2] Another example is a quantum support vector machine. Similar to qPCA, quantum support vectors rely on efficient preparation and exponentiation of density matrices that function as training data kernels.[4] This method makes use of the exponentiation of nonsparse Hermitian matrices that is introduced in the qPCA algorithm. For relatively non-complex machine learning tasks, qPCA is a good choice due to its simplicity and efficiency. For more complex tasks, the methods introduced in qPCA can be extended, as in the case of quantum support vectors, to perform more rigorous analysis.

4 Discussion

Quantum principle component analysis uses quantum states to perform a self-analysis eigen-decomposition to reveal its own structure. It provides a simple means of implementing QRAM to see exponential speed-up over classical algorithms. Primarily it is used to find eigenvectors corresponding to the largest eigenvalues for Hamiltonians. The complexity of the algorithm is close to linear and sublinear scaling of the sparse simulation is not feasible.

The paper by Lloyd, Mohseni, and Rebentrost is a landmark in the development of quantum machine learning and introduces techniques, particularly nonsparse matrix exponenti-

ation, that will be essential to many quantum machine learning algorithms. The algorithm is clearly presented and the techniques introduced have a broad applicability. Thus, it is deserved of publication. Quantum machine learning is a novel field of research and works such as this are laying the foundation for the utilization of quantum systems in addressing big data problems that remain beyond the scope of current technology.

References

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[4] Rebentrost, M. Mohseni, and S. Lloyd, "Quantum Support Vector Machine for Big Data Classification", Phys. Rev.Lett. 113, 130503 (2014).