Quantum Principal Component Analysis

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December 17, 2020

1 Introduction

Density Matrix Exponentiation

$$
\begin{aligned}
Tr_P(e^{-i\hat{S}\Delta t}\rho\otimes\sigma e^{i\hat{S}\Delta t}) &= Tr_P[\,(\cos\Delta t + i\hat{S}\sin\Delta t)\ \rho\otimes\sigma\ (\cos\Delta t - i\hat{S}\sin\Delta t)] \\
&\approx Tr_P[\,\rho\otimes\sigma - i\Delta t[\rho,\sigma] + O(\Delta t^2)] \\
&= \sigma - i\Delta t[\rho,\sigma] + O(\Delta t^2) \\
&\approx e^{-i\rho\Delta t}\ \sigma\ e^{i\rho\Delta t}
\end{aligned} \tag{1}
$$

Where Tr_P is the partial trace ρ over the first variable and $\hat{S}$ is the swap operator. Note that $\rho\otimes\sigma\hat{S} = \rho\otimes\sigma$. By repeating (1) n times,

$$
\begin{aligned}
&Tr_{P_1}Tr_{P_2}...Tr_{P_n}[\,e^{-i\hat{S}_n\Delta t}e^{-i\hat{S}_{n-1}\Delta t}...e^{-i\hat{S}_1\Delta t}(\rho^{\otimes n}\otimes\sigma)e^{i\hat{S}_1\Delta t}...e^{i\hat{S}_{n-1}\Delta t}e^{i\hat{S}_n\Delta t}] \\
&= Tr_{P_n}[\ e^{-i\hat{S}_n\Delta t}\ Tr_{P_{n-1}}[\,e^{-i\hat{S}_{n-1}}(...Tr_{P_1}[\,e^{-i\hat{S}_1\Delta t}(\rho^{\otimes n}\otimes\sigma)e^{i\hat{S}_1\Delta t}]\,)e^{i\hat{S}_{n-1}}]\ e^{i\hat{S}_n\Delta t}\ ] \\
&\approx e^{-i\rho n\Delta t}\ \sigma\ e^{i\rho n\Delta t}
\end{aligned} \tag{2}
$$

2 Two qubits case

Here, we use the quantum algorithm in Ref.[1] to perform PCA on a two features case, where the covariance matrix can be represented by a single qubit. The covariance matrix Σ and eigenvalues, e_1 and e_2, of the raw data provided in Ref.[1] are,

$$
\Sigma = \begin{pmatrix} 0.380952 & 0.573476 \\ 0.573476 & 1.29693 \end{pmatrix}, e_1 = 1.57286, e_2 = 0.105029. \tag{3}
$$

Now we are going to calculate e_1 and e_2 using quantum algorithm.

The first step is to calculate the $\hat{U}_{prep}$ classically which can prepare the two qubits pure state $|\psi\rangle$ from $|0\rangle$, where $|\psi\rangle$ is the purified state of Σ.

The second step is to prepare two copies of $|\psi\rangle$ on quantum computer by $\hat{U}_{prep}$. Note that $\hat{U}_{prep}$ can be decomposed as:

$$
\hat{U}_{prep} = (\hat{U}_A\otimes\hat{U}_B)CNOT_{AB}(\hat{U}'_A\otimes\hat{I}_B). \tag{4}
$$

Where $\hat{U}_i$ can be represented as,

$$
\begin{pmatrix} \cos(\theta/2) & -e^{i\lambda}\sin\theta/2 \\ e^{i\phi}\sin\theta/2 & e^{i\lambda+\phi}\cos\theta/2 \end{pmatrix}. \tag{5}
$$

The third step is to calculate the purity.

References

[1] P. J. Coles, S. Eidenbenz, S. Pakin, A. Adedoyin, J. Ambrosiano, P. Anisimov, W. Casper, G. Chennupati, C. Coffrin, H. Djidjev, et al. Quantum algorithm implementations for beginners. *arXiv*, pages arXiv–1804, 2018.