Quantum Principal Component Analysis

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1   Introduction

Density Matrix Exponentiation

$$Tr_P(e^{-i\hat{S}\Delta t}\rho \otimes \sigma e^{i\hat{S}\Delta t}) = Tr_P[\,(\cos\Delta t + i\hat{S}\sin\Delta t)\,\rho \otimes \sigma\,(\cos\Delta t - i\hat{S}\sin\Delta t)]$$

$$\approx Tr_P[\,\rho \otimes \sigma - i\Delta t[\rho,\sigma] + O(\Delta t^2)]$$

$$= \sigma - i\Delta t[\rho,\sigma] + O(\Delta t^2) \tag{1}$$

$$\approx e^{-i\rho\Delta t}\,\sigma\,e^{i\rho\Delta t}$$

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,

$$Tr_{P_1}Tr_{P_2}...Tr_{P_n}[\,e^{-i\hat{S}_n\Delta t}e^{-i\hat{S}_{n-1}\Delta t}...e^{-i\hat{S}_1\Delta t}(\rho^{\otimes n} \otimes \sigma)e^{i\hat{S}_1\Delta t}...e^{i\hat{S}_{n-1}\Delta t}e^{i\hat{S}_n\Delta t}]$$

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

$$\approx e^{-i\rho n\Delta t}\,\sigma\,e^{i\rho n\Delta t}$$

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 U_{prep} classically which can prepare the pure state $|\psi\rangle$ from $|0\rangle$, where $|\psi\rangle$ is the purified state of Σ.

The second step is to prepare $|\psi\rangle$ on quantum computer by U_{prep}.

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.