A Classical-Classical Approximation to Quantum State

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Abstract
Our research aims to quantify quantum discord in quantum states. We propose a numerical method based on minimizing the distance between a state and a set of zero quantum discord states. We introduce Stiefel manifolds to characterize the set and develop a descent flow algorithm that is reliable and consistent.

Introduction
Our goal is to quantify the level of quantumness in a given state, using a specific metric that applies to both entangled and separable states. Despite the difficulty of this problem, we are developing a numerical method to tackle it, as it is a critical factor in accelerating algorithms and communication in quantum systems.
We rely on the classical-classical approximation, which posits that a given classical-classical state can be expressed in the following form:

$$\sigma = \sum_i \theta_i (x_i x_i^T) \otimes (y_i y_i^T) = \sum_i \theta_i (x_i \otimes y_i\ ) \otimes (x_i \otimes y_i\ )^T,$$

where $\theta_i's$ are non-negative real numbers and unit sum; $\{x_i\} \subset H_A = R^n$and $\{y_i\} \subset H_B = R^m$ are orthonormal sets.

Problem Description
We will provide a brief explanation of how to find the nearest classical-classical state to a given quantum state. Specifically, we can formulate the optimization problem as follows for a given state ρ:

$$\text{find}\{x_i\},\{y_i\},\{\theta_i\}\ \text{that minimize} \left\| \rho - \sum_i \theta_i (x_i \otimes y_i\ ) \otimes (x_i \otimes y_i\ )^T \right\|_F^2.$$

Setting $U = [x_1, x_2, \cdots x_N], V = [y_1, y_2, \cdots y_N]$, and the orthogonality restriction which requires $U^T U = V^T V = I$.
Moreover, the Khatri-Rao product $\odot$ which $U \odot V = [x_1 \otimes y_1, x_2 \otimes y_2 \cdots x_N \otimes y_N]$enables us to rewrite the objective function as the following form:

$$\text{find } U, V, D = \{\theta_i\}\text{that minimize } F(U,V,D) = \frac{1}{2}\|\rho - (U \odot V)D(U \odot V)^T\|_F^2,$$
$$U^T U = V^T V = I_N,$$
$$Trace(D) = 1.$$

Gradient Flow
We derive the descent flow on the Stiefel manifolds $S_n = \{X \in R^{n\times N}, X^T X = I_N\}$ and $S_m = \{Y \in R^{m\times N}, Y^T Y = I_N\}$.
Let $(\frac{\partial F}{\partial U}, \frac{\partial F}{\partial U})$,be the Euclidient gradient of F with respect to U and V, the projections of given vectors onto S_n and S_m are defined as

$$Proj_{S_n}\left(\frac{\partial F}{\partial U}\right) = 2skew\left(\left(\frac{\partial F}{\partial U}\right)U^T\right)U,$$

$$Proj_{S_m}\left(\frac{\partial F}{\partial V}\right) = 2skew\left(\left(\frac{\partial F}{\partial V}\right)V^T\right)V.$$

Therefore, the descent flow on Stiefel manifolds can be derived as

$$\frac{\partial U}{\partial t} = -Proj_{S_n}\left(\frac{\partial F}{\partial U}\right),$$
$$\frac{\partial V}{\partial t} = -Proj_{S_m}\left(\frac{\partial F}{\partial V}\right).$$

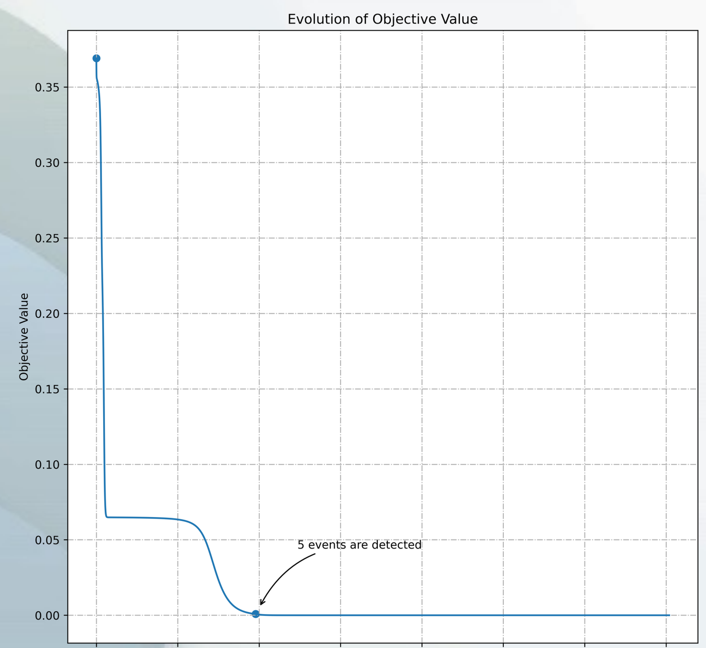
The descent flow of θ_i is given in the following form,

$$\frac{\partial \theta_i}{\partial t} = -\left(e_i - \frac{1}{N}\sum_i e_i\right),$$

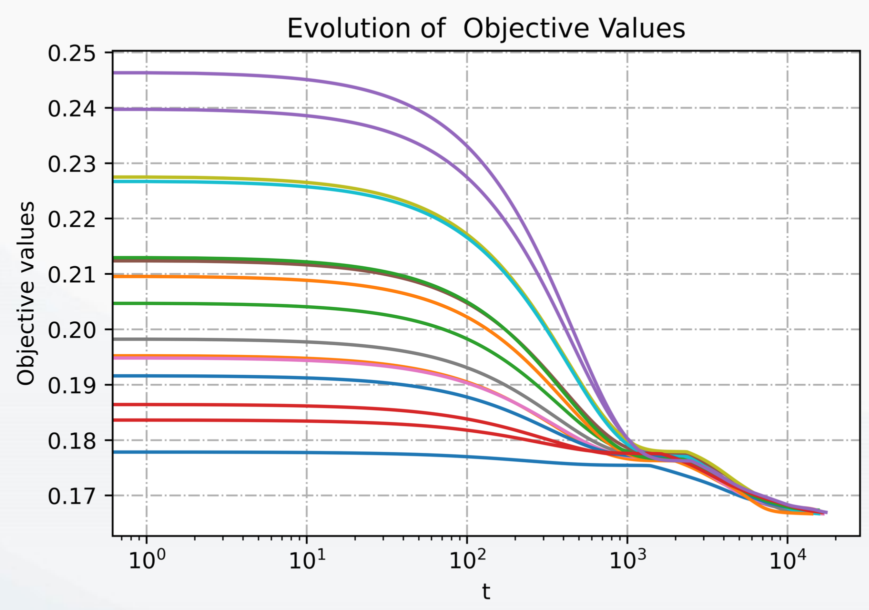
where $e_i = \theta_i\ - <\rho, (x_i \otimes y_i\ ) \otimes (x_i \otimes y_i\ )^T>.$

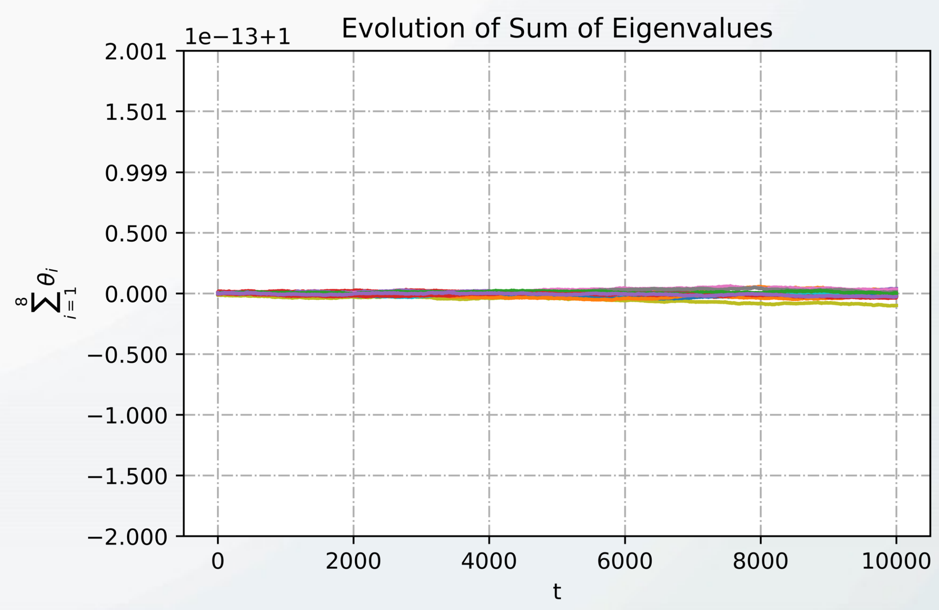
Numerical Results
We will evaluate whether our method satisfies two key criteria: First, whether it can accurately recover a classical-classical state, and second, whether it is robust to variations in the initial conditions.

Experience 1
demonstrates the method's capacity to retrieve a specified classical-classical state.



Experience 2
Verifies that the sum-to-one property is preserved and demonstrates that the optimal function value is independent of the initial condition.





Conclusion
In conclusion, our study focused on quantifying quantum discord in quantum states, and we proposed a numerical method to achieve this goal. Our approach involved minimizing the distance between a given state and a set of zero quantum discord states, characterized by Stiefel manifolds. We developed a reliable and consistent descent flow algorithm to solve this optimization problem. Additionally, we demonstrated the effectiveness of our approach by solving the classical-classical approximation of a given state using an ODE system and presented numerical examples to showcase its properties. Overall, this study is just the start of the exciting journey into quantum computation.

[1] B.Z Lu, Y.C Su, M.M Lin, Approximation of the Nearest Classical-Classical State to a Quantum State, *preprint, arxiv* https://arxiv.org/abs/2301.09316
[2] M.T Chu, M.M Lin, A complex-valued gradient flow for the entangled bipartite low rank approximation, *Computer Physics Communications*, 271 (2022), 108185.