QAOA ansatz and differential evolution for quantum molecular comparison

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Abstract

The perception of tastes and sensations: sweet, sour, bitter, acid, salty, umami, but also freshness, cold, warmth, and even carbonation, amongst others, is mediated by different receptors. With a virtual screening (VS) method implemented and refined for quantum gate-based computation, we can predict whether a molecule binds adequately to the freshness receptor, activating the transmission signal that indicates the freshness sensation to the brain. The aim is to design, before consumption, tailor-made food and beverage products.
The VS method used determines the maximum common substructure between molecules, mappable to the maximum-weighted set problem over a conflict graph, where the edges are conflicts to avoid. For this case, we implement a weighted variation of the original QAOA with (1+n) parameters per layer inspired by the ma-QAOA [1], being n the number of qubits. We choose differential evolution as the optimiser since it evades local minima [2]. With two layers, we find optimal configurations until 19 qubits through emulation with standard deviations of upper order 0.1 (Figure 1).

References

[1] Herrman, R., Lotshaw, P.C., Ostrowski, J. et al. Multi-angle quantum approximate optimization algorithm. Sci Rep 12, 6781 (2022).
[2] Faílde, D., Viqueira, J.D., Mussa Juane, M. et al. Using Differential Evolution to avoid local minima in Variational Quantum Algorithms. Sci Rep 13, 16230 (2023).

Figures

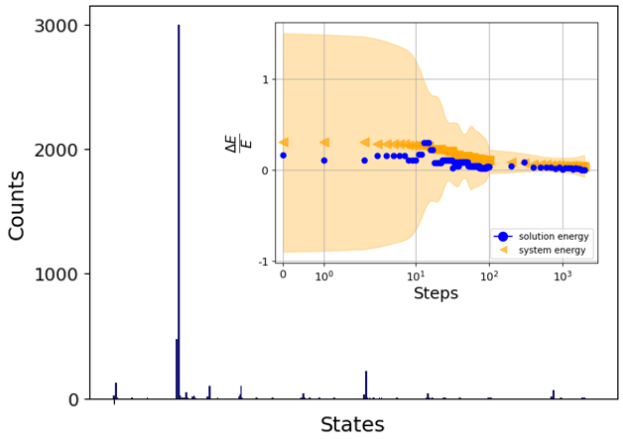

Figure 1: Final distribution with 3000 out of 10000 counts for the optimal configuration with 0 conflicts (molecule a-cedrene with 19 qubits). Embedded, energy evolution of the optimal configuration with its standard deviation and of the whole system.

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