A probabilistic perspective for optimizing the parameters of quantum heuristics using evolutionary algorithms

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ABSTRACT

Variational quantum algorithms (VQAs) (Cerezo et al. [2021]) are hybrid approaches between classical and quantum computation, where a classical optimizer proposes parameter configurations for a quantum parametric circuit which is iteratively measured. Each measured solution is assessed according to a cost function that evaluates the energy of the system, which is sought to be optimized. The performance of the VQA heavily depends on how the classical optimizer tunes the parameters, and also on the number of sequential layers of the quantum parametric circuit.

Estimation of distribution algorithms (EDAs) (Larrañaga and Lozano [2001]) are a type of evolutionary algorithms where a probabilistic model is updated and sampled at each generation to optimize a cost function. Depending on the restrictions of the probabilistic model embedded in the EDA, a wide range of variants are identified, such as the univariate marginal distribution algorithm (Mühlenbein et al. [1996]), which uses independent Gaussians, the estimation of Gaussian network algorithm (Larrañaga et al. [2000]), which uses multivariate Gaussian Bayesian networks, and the semiparametric estimation of distribution algorithm (Soloviev et al. [2022a]), where a coexistence of Gaussian and kernel density estimated probability distributions are allowed within Bayesian networks. The use of a univariate case of the EDAs for the VQA parameter tuning has been used achieving successful results compared to other approaches and is available in Qiskit (Soloviev et al. [2022b]).

In this work, we perform a comparison of the different EDA variants for the parameter tuning of two different VQAs: the quantum approximate optimization algorithm (Farhi et al. [2014]), and the variational quantum eigensolver (Peruzzo et al. [2014]). The results show competitive results of the different EDAs compared to some gradient-based and gradient-free optimizers, typically used in the literature, and identify which characteristics of the problem fit better to each variant.

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