Training embedding quantum kernels with quantum neural networks

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ABSTRACT

Recent years have seen significant advancements in implementing supervised machine learning on quantum processors. While parametrized quantum circuits are the most prevalent approach, kernel methods play a pivotal role in comprehending quantum machine learning models and have the added advantage of guaranteeing smaller labeling errors. Within the realm of quantum kernels, embedding quantum kernels (EQK) are derived by evaluating inner products between quantum feature states with the primary challenge selecting the appropriate embedding, as the effectiveness of a EQK is contingent on the specific learning task. However, techniques of training EQKs from parametrized embedding ansatzes involve computing the kernel matrix, incurring a quadratic complexity in the number of training samples, at every training step. In response, we propose the utilization of a n-qubit Quantum Neural Network (QNN) based on data re-uploading to identify the optimal $m \cdot n$-qubit EQK for a task (n-to-$m \cdot n$). This method requires constructing the kernel matrix only once, offering improved efficiency. We illustrate our EQK protocol through two scenarios: n-to-n, where we propose a scalable approach to train an n-qubit QNN, and 1-to-n, demonstrating that the training of a single-qubit QNN can be leveraged to construct powerful EQKs tailored for the NISQ era. This is based on the work from Ref. [1].

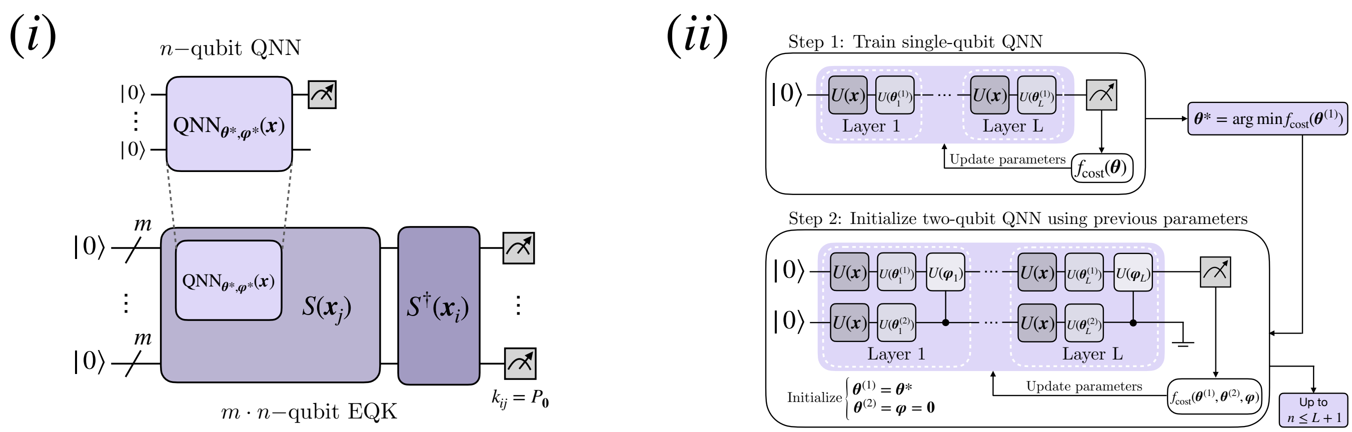

FIG. 1. (i) Overview of the construction proposed in this work. A quantum neural network of n qubits is subsequently used to build a $m \cdot n$-qubit embedding quantum kernel. (ii) Iterative training of a two-qubit data re-uploading QNN. In Step 1, a single-qubit QNN is trained to obtain optimal model parameters denoted as $\boldsymbol{\theta}^*$. Moving to Step 2, training for the two-qubit QNN is initiated, initializing new extra parameters to 0, while the parameters of the first qubit are set to $\boldsymbol{\theta}^*$. This iterative approach can scale the QNN up to $n \leq L + 1$ qubits, ensuring that the n-qubit QNN performs at least as effectively as the $n - 1$ version.

We propose a method for constructing trained embedding quantum kernels (EQK) using quantum neural networks (QNN). The idea is depicted in Figure 1 (i) and consists of training the n-qubit QNN for a classification task and leveraging its architecture to generate $m \cdot n$-qubit EQKs tailored to the specific task, calling this construction n-to-$m \cdot n$, thereby enhancing performance on the given dataset. In particular, we focus on two cases: the n-to-n and the 1-to-n scenarios. The motivation for combining these two binary classification approaches, QNN and kernel methods, arises from two perspectives.

Firstly, we investigate whether the QNN can effectively select a suitable embedding kernel for a specific task. This approach may lead to more efficient kernel training compared to previous methods, as we only need to construct the kernel matrix once. Secondly, the QNN's performance is contingent on its training. Utilizing the corresponding EQK construction might produce superior results compared to relying solely on the QNN, even in cases where the training process has not been optimal.

In our approach, we adopt a data re-uploading-based architecture for QNN. Recognizing the non-trivial nature of training parametrized quantum circuits, we introduce a novel iterative scaling technique.

For the training of the n-qubit QNN, we propose an iterative construction starting from a single-qubit QNN. The initialization process is depicted in Figure 1 (*ii*). Initially, we train a single-qubit QNN and utilize its parameters to initialize the two-qubit QNN. During the initialization of the two-qubit QNN, we set $\varphi_l^{(1)} = \mathbf{0}$ for all $l \in [1, L]$, initializing the parameters of the first qubit with those obtained from the training of the single-qubit step. Consequently, the entangling layers do not have any action, ensuring that, with a local measurement on the first qubit, we commence in the output state of the single-qubit QNN training.

This process can be employed to scale up the QNN architecture, allowing the construction of QNNs with up to n qubits. When adding an extra qubit, the supplementary entangling gates are initialized as identities, and the training begins with the optimal parameters obtained from the previous step. Essentially, this formalized approach signifies a systematic and scalable improvement in the QNN's performance with the incorporation of each additional qubit.

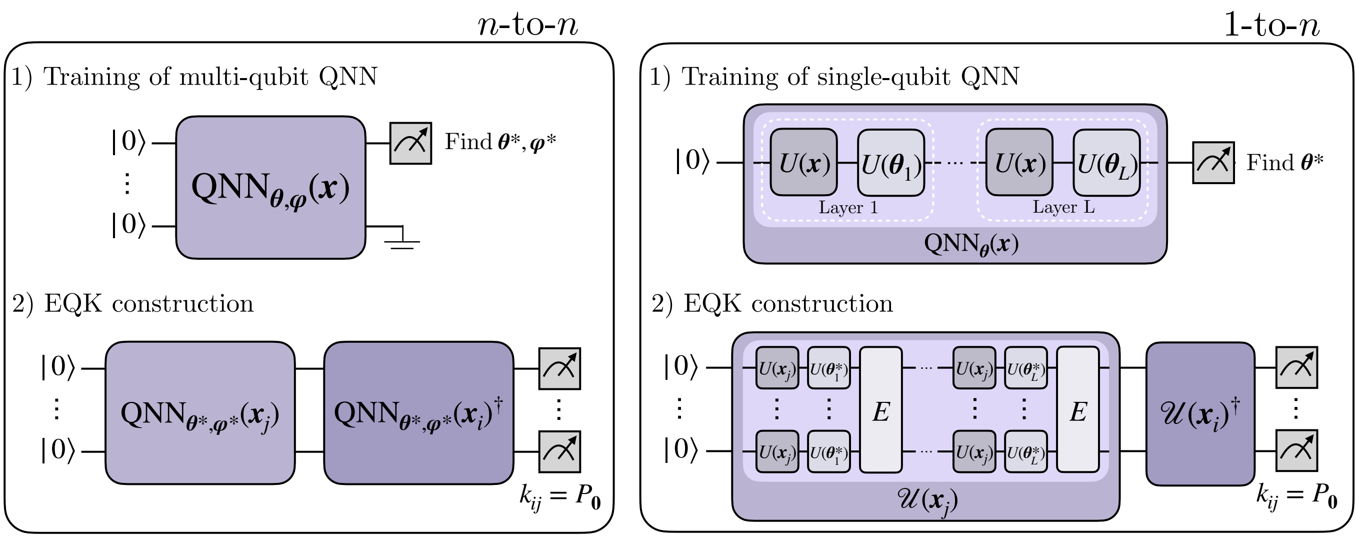

FIG. 2. Embedding quantum kernels generated from quantum neural networks training. The kernel matrix element k_{ij} is defined as the probability of measuring all qubits in the state $|0\rangle$, denoted as $P_{\mathbf{0}}$. On the left, we have the n-to-n proposal, constructed by directly utilizing the trained data re-uploading n-qubit QNN as a quantum feature map. On the right, we show the construction of an Embedded EQK from the training of a single-qubit QNN, named as 1-to-n.

In our construction, it is true that when the QNN is optimally trained, the improvement from introducing the EQK construction is minimal. However, we observe that even when the QNN training is suboptimal, the performance of the corresponding EQK remains as high as in the optimal case. This suggests that only a few training iterations for the QNN are sufficient to select a suitable embedding for constructing a robust EQK. While achieving optimal QNN training is generally straightforward for systems with few qubits, as these systems are classically simulable, the robustness of the EQK becomes crucial when dealing with larger quantum machine learning models where optimal training is not guaranteed. In such cases, you can attempt to train the model as extensively as possible and then leverage the architecture to construct an EQK.

This is demonstrated in the numerical results shown in Figure 3, which is based on a real-world data classification problem involving the identification of solar panels in satellite images. On the left, we see an optimally trained QNN leading to a two-qubit EQK. The enhancement in this case is not substantial. However, on the right, we intentionally train the QNN sub-optimally, yet the performance of the corresponding EQK remains the same, demonstrating the robustness of our approach.

[1] P. Rodriguez-Grasa, Y. Ban, and M. Sanz, "Training embedding quantum kernels with data re-uploading quantum neural networks," (2024), arXiv:2401.04642 [quant-ph].

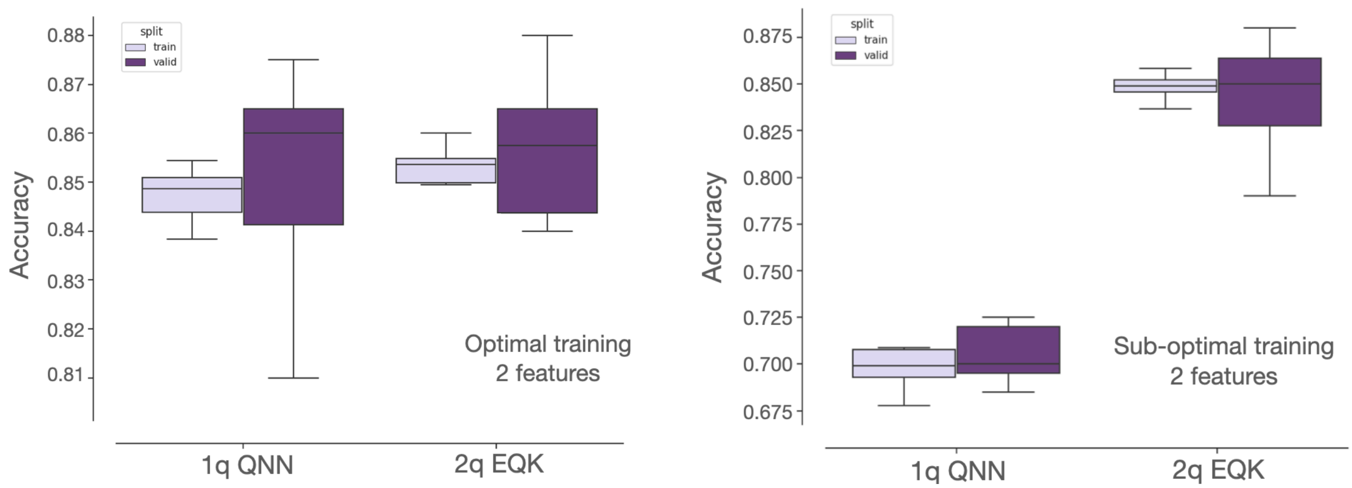

FIG. 3. Test accuracies for a real-world data classification problem using a single-qubit QNN and leveraging this architecture to create an EQK as proposed in our work. On the left, the QNN is optimally trained, while on the right, we reduce the number of training epochs to intentionally achieve sub-optimal training.