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Evaluating Variational Quantum Circuit Designs for Knowledge Graph Completion

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***Abstract*—Knowledge graphs (KGs) are informative knowledge bases for various applications such as semantic web search or question answering. Since KGs often have missing facts mainly due to large construction costs, KG completion is a fundamental problem. Nowadays, as KGs have become large-scale, KG completion has become gradually intractable for classical computers. One promising direction is to utilize quantum circuits to capture complex structural information that entities and relations in KGs have. By encoding entities into quantum states and representing relations between entities as quantum circuits running on the quantum states, it becomes able to score and predict plausible missing entities or relations. However, it is still unclear how to design the quantum circuits to enhance KG completion accuracy. In this paper, we evaluate variations of quantum circuits in terms of KG completion accuracy, and investigate the relationship between the accuracy and the quality of the circuits (e.g., expressibility and entangling capacity). The experiments using a real KG show some correlation between the completion accuracy and the goodness of the circuits.**

***Index Terms*—Knowledge graph, Knowledge graph completion, Quantum circuits, Expressibility, Entangling capacity**

I. Introduction

Quantum computers have attracted much attention as computing systems efficient for combinatorial information. Knowledge graph (KG) is a famous format of human knowledge bases made of combinations of entities and relations. For example, "Tokyo" and "Japan" are the entities, and "capital of" is the relation between the above entities.

Since existing KGs are manually made and thus incomplete subsets of true combinations of entities and relations, a fundamental problem for KGs is to predict unseen combinations of entities and relations. This problem called "KG completion" has been tackled in machine learning fields using classical computers. However, it has become gradually intractable for classical computers according to the growth of KGs.

In classical machine learning, a standard way to handle combinatorial information in KG is to embed entities onto vector space and then to score the combination with a relation by some scoring functions. On the analogy of the classical machine learning method, quantum machine learning can embed entities as quantum states and score the combination with a relation using some quantum circuits. It can be expected that a small number of qubits and a quantum circuit over the qubits can express complex structure of human knowledge more efficiently than the classical one. Some leading studies [2], [3] have shown the potential. However, how to design the quantum circuit to improve KG completion is still unclear.

In this paper, we design a template of quantum circuit for KG completion and evaluate KG completion accuracy for 18 circuits, following some existing studies. Then, we investigate the relationship between the accuracy and the goodness of the circuits,e.g., expressibility and entangling capacity, and found some correlation.

II. Related work: KG completion

Typical machine learning-based methods are two types: translation models and factorization models. Translation models assume a vector operation to characterize each triple containing a head, a relation, and a tail, denoted as (h, r, t). TransE [1] assumes $\boldsymbol{h} + \boldsymbol{r} \sim \boldsymbol{t}$ for the corresponding vectors $\boldsymbol{h}, \boldsymbol{r}, \boldsymbol{t}$. Later works such as RotatE [6] have improved relational representations.

Factorization models assume an matrix operation M_r to characterize the relation between entities. RESCAL [4] formulates the scoring function as $\boldsymbol{h}^T M_r \boldsymbol{t}$. DistMult [7] is correspondent to the case where only every diagonal element of M_r is a free parameter. Y. Ma et al. [2], [3] extended factorization models to employ quantum machine learning algorithms but evaluated only a few variations of circuits.

III. Quantum circuit design and evaluation

Figure 1 illustrates the template of our quantum circuit for KG completion. This template basically follows Y. Ma et al. paper [2]. This circuit represents a factorization model $\langle h|Q_{h,r,t}(\Theta_h, \Theta_r, \Theta_t)|t\rangle$ in which head states $|h\rangle$ and tail states $|t\rangle$ are correlated with a triple-related operation $Q_{h,r,t}(\cdot)$. More precisely, a head circuit $Q_{h,r}(\Theta_h, \Theta_r)\,|h\rangle$ and a tail circuit $Q_t(\Theta_t)\,|t\rangle$ are separately run and the final swap test measures the norm of both results. The difference between the template and Y. Ma et al. paper is that we generalize each block denoted as $Q(\cdot)$ so that we can assign any general circuit to $Q(\cdot)$. We try 18 types of circuits (circuit 2-19) appeared in [5] for $Q(\cdot)$. We eliminate the circuit 1, for the circuit is fully not-entangled.

For evaluating KG completion accuracy, we use the proportion of correct answers ranked in top-10 (Hits@10). For

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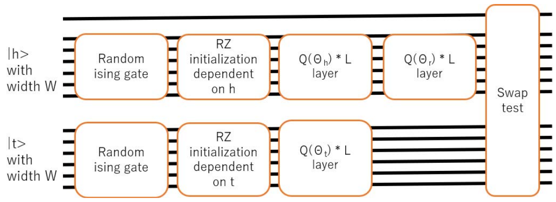

Fig. 1. Quantum circuit design for KG completion

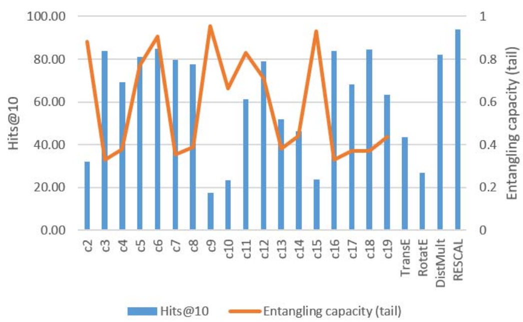

Fig. 2. Performance of KG completion

measuring the quantum circuit quality, we use the following measures:

- **Expressibility** [5] (for head and tail circuits) is (the lower, the better) measure of how well each quantum circuit can represent the corresponding Hilbert space.
- **Entangling capability** [5] (for head and tail circuits) is defined as the average of Meyer-Wallach entanglement of states, generated from the sample of parameters of each parameterized quantum circuit.
- **Circuit depth** is the total number of time slices required to finish each circuit $Q(\cdot)$.
- **h, rx, ry, rz, cnot, cz, crx, crz** is a binary indicator which indicates whether the circuit includes the corresponding gate.

IV. Experiments and Discussion

1) Dataset: We evaluate using kinship dataset [8] which contains two family members as entities and relations between them. The number of entities, relations, and triples is 104, 25, and 9,617, respectively. We held out 1,069 triples for test data, and we use the rest triples for training data.

2) Experimental settings: We set head and tail circuit width (qubits) $W = 6$, and build a $L = 3$ layer model. Quantum calculation is made by a quantum simulator using PennyLane-Lightning. Parameters are optimized using Adam algorithm with a learning rate as 0.001. The embedding dimension of classical models is set as $2^6 = 64$. We run 5 epochs for training due to time limitation.

3) Experimental results and discussions: Figure 2 shows the KG completion accuracy (Hits@10) based on the circuit 2-19 (c2-19). The best score among them is 85.03 (c6), which outperforms classical methods except RESCAL the score of which is 94.01.

Figure 2 also shows the entangling capacity of each circuit. We cannot find direct correlation with KG completion accuracy, so we use linear regression model to predict KG completion accuracy by the circuit (max-min scaled) characteristics. In this analysis, we conducted leave-one-out cross validation. The resulting R^2 score was 0.881. For example, the resulting model to predict the completion accuracy of the circuit 6 is below:

- Intercept: 15.86
- Coefficients:
  - Expressibility(head, tail): 4.93, 14.4
  - Entangling capacity(head, tail): -71.1, 31.7
  - Circuit depth: 62.9
  - h, rx, ry, rz, cnot, cz, crx, crz: 27.8, -12.5, 12.5, 64.2, -0.439, 9.41, -0.406, -4.90

Among the circuit characteristics, depth and rz gates have positive effect for the KG completion accuracy, which might suggest high depth leads better representation but dependence on rz gates might be caused by circuit design bias. While the entangling capacity of the tail circuit has positive effect, the entangling capacity of the head circuit has negative effect, which might suggest the discrepancy between the entangling capacity between head and tail circuits causes negative effect, i.e. asymmetric design of both circuits is not good.

V. Conclusion and Further Study

In this paper, we investigate the relationship between the KG completion accuracy and the quality of quantum circuits. In the future, we should conduct more experiments to find out whether the suggestion made in this study is valid.

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