

Quantum assisted unsupervised data clustering on the basis of neural networks

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Unsupervised machine learning is one of the main directions in the area of artificial intelligence. Here, we propose a realization of quantum assisted unsupervised data clustering on the basis of artificial neural network called a self-organizing feature map. We make a proof-of-concept realization of one of the crucial parts of the approach on IBM quantum machine and show that it allows us to reduce number of calculations in a number of clusters. We compare the results with the classical algorithm on a toy example of unsupervised text clustering.

I. INTRODUCTION

The combination of big data and artificial intelligence — dubbed the fourth industrial revolution — has profoundly affected the modern economy in a plethora of different ways from robotics to agriculture [1–5]. Contemporary artificial intelligence methods based on neural networks also have the potential to enhance the role of novel analytical methods in science and engineering [6–8]. Paradoxically, the exact mechanism of why neural networks are so powerful are remain unknown (in many cases it is regarded as a black box). It has been speculated that limits to the neural network approach based on the computational power of von Neumann architecture are being approached, and improvements appear only due to heuristic escalation of complexity. [TB: reference?] In particularly, the self-organizing feature map (SOFM) [9–11], is a type of artificial neural network (ANN) that is trained in an unsupervised manner. SOFMs are used in many areas [12–19] and in comparison with many other artificial neural networks they apply competitive learning and preserve the topological properties of the input space [20]. The SOFMs with a small number of nodes are

similar to the K-means algorithm but for larger SOFMs they represent data in a fundamentally topological way that allows one to do dimensionality reduction. Once it is trained, the map can classify a vector from the input space by finding the node with the smallest distance metric.

Meanwhile, there has been much interest recently in applying quantum computing techniques to machine learning [21–27]. [TB: I think you need to expand this paragraph a bit more, talk about related examples specifically, and don't just put a list of references] Quantum machine learning protocols utilize quantum phenomena including quantum entanglement and quantum superposition to tasks such linear regression and principal component analysis. [TB: please put references] Quantum machine learning approaches have the potential to outperform classical algorithms in many specific problems, in particular, many approaches for realizing quantum neural networks were proposed recently [28–39]. [TB: Since you use QAOA, I think you should talk about that a bit more here too, so that it can be easily introduced in the next paragraph]

In this paper, we realize a hybrid quantum assisted SOFM (QASOFM) and apply it to the data clustering problem in an unsupervised manner on a toy example of clustering paper abstracts (see Fig. 1). [TB: Explain the

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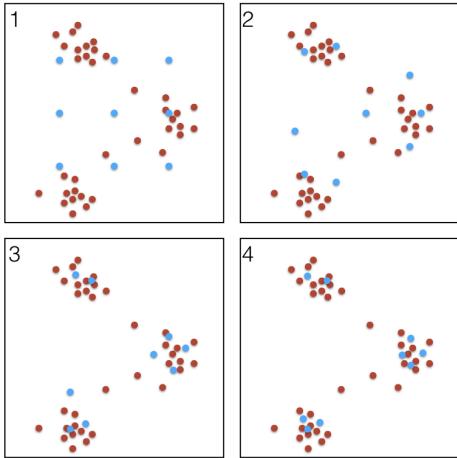


FIG. 1. Schematic illustration of the clustering problem considered in this paper. Blue dots represent clusters and red dots are data points. The training process moves clusters to fit the data points. Note that there are fewer clusters than data points which is the essence of dimensionality reduction and is what permits the model to generalize the data. [TB: Can you briefly talk about the QAOA aspect here, where it is calculated?]

figure a bit here, so we can get the general idea] We implement the quantum assisted SOFM in such a way that it becomes possible to use the Hamming distance as a distance metric for the training and to reduce the number of distance calculations in the number of clusters. We propose an optimized circuit for realizing the Hamming distance on a quantum machine. We prepare a toy example of data for clustering paper abstracts and give a proof-of-concept realization of the quantum assisted SOFM on the IBM Q experience quantum computer [40] and compare it with the classical case.

II. THE QUANTUM ASSISTED SELF-ORGANIZING FEATURE MAP (SOFM)

SOFM is one of the best-known unsupervised learning methods that is widely used in various areas of modern science. It was first proposed by Kohonen as a self-organizing unsupervised learning algorithm which produces feature maps similar to those occurring in the brain. [TB: reference] The SOFM algorithm operates with a set of input objects, each represented by a N -dimensional vector, as input and maps them onto nodes of a two-dimensional grid.

The input dimensions are associated with features and nodes in the grid, called cluster vectors, are assigned the N -dimensional vectors; the components of these vectors are usually called weights. Initially weight components are chosen randomly. We then can train our SOFM adjusting the components through the learning process which can be oversimplified into two basic procedures, selecting a winning cluster vector and updating its weights

(Fig. 1). In more detail, they consist of four step process: 1) select an input vector randomly from the set of all input vectors; 2) find a cluster vector which is closest to the input vector; 3) adjust the weights of the winning node in such a way that it becomes even closer to the input vector; 4) repeat this process many iterations until it converges [MN: I think we should say something more about the convergence criterion, make it more formal, especially that later we say "convergence is already observed in the fourth epoch"].

After the winning cluster vector is selected, the weights of the vector are adjusted according to

$$\vec{w}_{\text{new}} = \vec{w}_{\text{old}} + \alpha (\vec{x} - \vec{w}_{\text{old}}). \quad (1)$$

In simple words, this expression can be understood according to the following: if a component of the input vector is greater than the corresponding weight, increase the weight by a small amount; if the input component is smaller than the weight, decrease the weight by a small amount. The larger the difference between the input component and the weight component, the larger increment (decrement). [MN: this description - although accurate - I don't think is sufficient to grasp the intuition of what is going on, I think it would be very useful to a description of how to build a geometrical interpretation of the process, after all updating weights is moving the vectors in space, we could clarify this here and reference to figure 1 and it should resolve the confusion about the figure as well.]

Intuitively, this procedure can be geometrically interpreted as iteratively moving the cluster vectors in space one at a time in a way that ensures each move is following the current trends inferred from their distances to the input objects. A visualisation of this process is provided on figure (Fig. 1).

The process continues until [MN: here I would explain the formal convergence criterion] criterion is met.

Usually the winning cluster vector is selected based on the Euclidean distance between an input vector and the cluster vectors. In our approach, we use the Hamming distance instead of the Euclidean distance to select the winning cluster vector. It allows us to use a simpler encoding of the classical information into the quantum state and use an effective procedure for the calculation of the Hamming distance on the quantum machine, such as to reduce the number of calculations in number of cluster vectors in comparison to the classical case.

A. Optimized quantum scheme for Hamming distance calculation

We now introduce an optimized algorithm for calculating the matrix of Hamming distances [41] between a sample vector and all cluster vectors at once. This allows for a simple encoding of the classical information into a quantum register. Initially we have two registers each

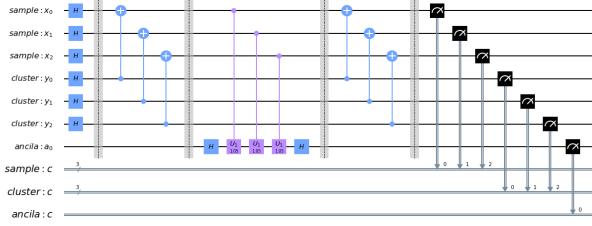
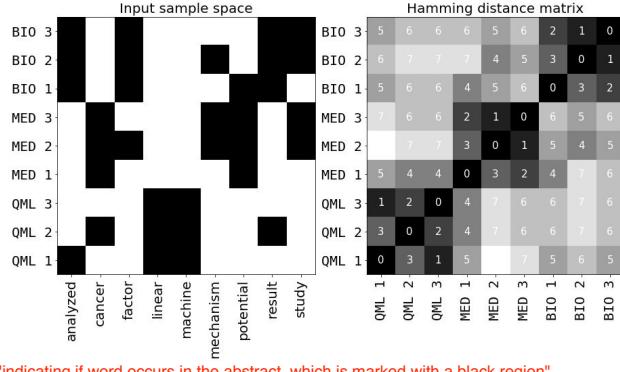


FIG. 2. A quantum circuit for the Hamming distance calculation algorithm between all samples and clusters at once. First, we apply Hadamard gates in order to get superposition of the sample and cluster registers. Second, we encoded information about pairwise different qubits in a quantum state of the sample register with applying the CNOT gates. Third, Hamming distance values are encoded in the amplitudes of superposition with the control phase rotation and Hadamard gates. Finally, a quantum state of the sample register returned to the initial basis for information retrieval.



"indicating if word occurs in the abstract, which is marked with a black region"

FIG. 3. [TB: can you label the figures by (a) and (b) and write the corresponding caption.] (a) Representation of the data set of abstracts with the bag-of-words model is shown. Each abstract is represented by a binary vector with 9 elements. The samples are sorted into groups (QML, MED, BIO), 3 papers for each tag. (b) The Hamming distance between each vectorized abstract is shown with a number in the matrix. The sets of abstracts are well separated.

mention in caption that this data set would correspond to red dots from fig 1.

with n qubits in that we encode our set of binary vectors defined as

$$|X\rangle = \sum_{i=1}^k |x_i\rangle, \quad (2)$$

$$|Y\rangle = \sum_{i=1}^l |y_i\rangle, \quad (3)$$

where $1 \leq k, l \leq n$. Here the registers $|X\rangle$ and $|Y\rangle$ correspond to the input states and the cluster states respectively. The initial state of whole circuit is

$$|\psi_0\rangle = |X\rangle |Y\rangle |a\rangle \quad (4)$$

where $|a\rangle$ is an auxiliary qubit. [TB: I removed the n superscript, I think it can be implicit] We then apply a

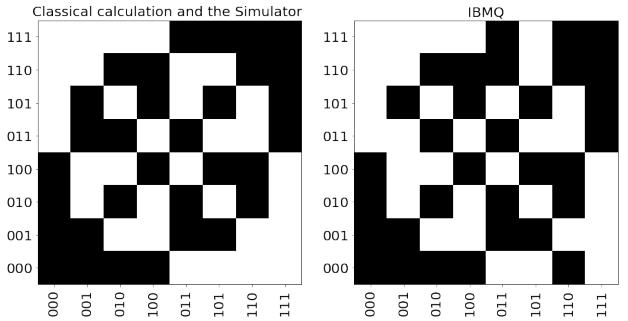


FIG. 4. The Hamming distance matrix between data sets of binary vectors. Values of distance that **less than** median distance value was marked black. The classical simulation of the quantum circuit shows perfect agreement to theoretical calculations and presented on the left figure. Result obtained on IBMQ "ibmq_16_melbourne" backend is shown on the right figure. **mention in this caption that this data set is an example data set and it is meant to show agreement of output with the quantum algorithm with the classical one**

CNOT gate between $|X\rangle$ and $|Y\rangle$

$$|\psi_1\rangle = \left(\sum_{i=1}^n \text{CNOT}(|Y\rangle_i, |X\rangle_i) \right) |a\rangle \quad (5)$$

[TB: How is $|Y\rangle_i, |X\rangle_i$ defined? We defined only $|x_i\rangle$. Can you make this clearer?] In the result, we encoded information about pairwise different qubits in $\{X\}$ and $\{Y\}$ into register $|X\rangle$. After this step we transfer information about the distance between the sample state and the cluster state into the amplitude of the superposed state. In order to do this we apply a Hadamard gate on the auxiliary qubit, then the controlled phase gate on $|a\rangle$ with the control being $|X\rangle^n$. The controlled phase gate is defined as

$$R(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{-i\phi} \end{pmatrix}, \quad (6)$$

where $\phi = \frac{\pi}{n}$. Finally a Hadamard gate is applied again. [TB: Maybe its better just to draw a quantum circuit which shows all the steps? I know you have Fig. 2 but this is the full circuit, maybe something more minimal to show the procedure.]

This returns us to our initial basis for register $|X\rangle^n$

$$|\psi_1\rangle = \left(\sum_i^n \text{CNOT}(|Y\rangle_i^n, |X\rangle_i^n) \right) |a\rangle \quad (7)$$

In comparison with the circuits for Hamming distance calculations proposed previously, our method allows one to reduce number of gates in the circuit and can be implemented with higher fidelity on current quantum devices. [add comparison of complexities in number of gates for realization between our scheme and previously proposed schemes (one qubit and two qubit separately)]

mention in this caption that the cluster vectors on top left (a) would correspond to initial blue dots on fig 1 and bottom left to final configuration of blue dots from fig 1,

mention somewhere that our approach cannot be visualized in the same way as fig 1. because bag of words contain many words translating to more than three dimensions and also coordinates are binary (word belongs to abstract or not)

III. DEMONSTRATION OF QASOFM ON THE IBM Q EXPERIENCE

We now show results for a proof-of-concept demonstration of the algorithm introduced in the previous section, on a 16-qubit quantum computer provided by IBM Q Experience. We implement unsupervised data clustering for three sets of paper abstracts from three different fields: quantum physics [42–44], medicine [45–47] and biology [48–50]. Each set consists of three random papers that focus on one of following topics: “Quantum Machine Learning” (QML), “Cancer” (MED) and “Gene Expression” (BIO). Abstracts were vectorized by the bag-of-words model in order to choose most defining words in each data set (see Fig. 3). This model represents text as a multiset “bag”) [MN: I replaced a ‘set’ with ‘multiset’ as pure sets due to (one of) my reasons lack of possibility of repeating elements cannot be used to represent text] of its words taking into account only multiplicity of words. Preparing the bag-of-words we excluded the words that appear only in one abstract and more than in 4 abstracts and we also excluded the word “level” from consideration due to the frequent overlap between the clusters because it gives instabilities for both classical and quantum algorithms. We restricted our bag-of-word size to 9 of the most frequent words from the full “bags-of-word” due to limitations of the number of qubits. [TB: correct?] After vectorizing and pre-processing the data, clusters are well separated with the Hamming distance. We observe that distances between the abstracts inside clusters are smaller than distances between the abstracts from different clusters, showing a successful self-organization (Fig. 3).

Classical SOFM [9], as it has been explained earlier, can be oversimplified into two basic procedures [MN: I changed the wording here for consistency]: distance calculation between a sample vector and all clusters vectors and shifting the closest cluster vector to the sample vector. In classical SOFM, the complexity of algorithm in the sense of number of distance calculations scales as $O(LMN)$, where N is number of samples, M is number of randomly sampled cluster vectors, and L is number of the shifts of cluster vectors. In the QASOFM (Sec. II), distance calculations are realized on a quantum device (i.e. the IBM Q Experience) with the use of circuit presented in Fig. 2. This approach allows one to reduce the number of operations in a number of cluster states with an optimized number of gates that are possible to realize on currently available quantum computing devices with a limited number of qubits. The circuit realized in such a manner that calculation of Hamming distance between the sample vector and all cluster vectors is realized in one operation. The complexity of the quantum assisted SOFM then scales as $O(LN)$.

In order to check that our algorithm gives the correct results we compare it to classical calculations of the distance matrix, as shown in Fig. 4. We see good agreement between the distance matrices calculated classically and

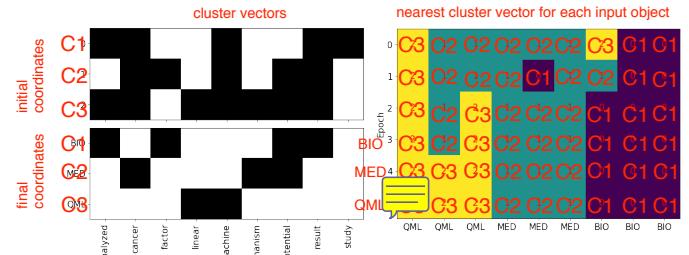


FIG. 5. [TB: Please add subfigure labels (a)(b)(c). (a) Initial random binary vectors of clusters are presented. We randomly sampled 3 binary vectors of size 9 as initial cluster vectors (labeled by 0,1,2) and it is shown how the words from the bag of words model presented in them. The result of applying our QASOFM implemented on the IBMQ “ibmq_16_melbourne” backend is shown on the bottom left figure. Vectors mean cluster elements for BIO, MED, QML groups, respectively (up to down). The evolution of label distribution on each learning epoch is presented on the right figure. Good convergence already is observed on the fourth epoch.

mention in this caption that the input objects are not visualized on TH but they are on fig 3.

on the IBM Q Experience. The theoretical calculations and classical simulations show perfect agreement with each other. An example of the QASOFM learning process is given on Fig. 5. Initially, the cluster vectors were randomly chosen (see Fig. 5) and label of sample distribution is shown for the zeroth epoch in Fig. 5(b). In order to prepare a superposition of cluster vectors needed for the calculation of the distance matrix at once we use the standard initialization of QISKit library. Each epoch of the algorithm requires 9 distance calculations in the quantum implementation (number of samples in general case) or 27 distance calculations for classical realization (product of number of samples and number of cluster vectors in general case). In order to realize the circuit for the distance calculation for the quantum case we used the IBM Q machine. After the distance calculation from each sample to all cluster vectors at each epoch we label each sample with the index of the closest cluster vector and shift the closest cluster vectors to the sample one. The shift is made by the change of the first binary element in the cluster vectors different from the sample one. The evolution of the labels presented on Fig. 5(b). Good convergence is already observed in the fourth epoch.

IV. DISCUSSIONS

We have developed a quantum assisted SOFM and showed a proof-of-concept demonstration that it can be used to solve clustering problems in an unsupervised manner with potential to outperform classical counterpart in real life tasks. The procedure of solving such clustering problem requires calculating the distance many times in iterative way. We introduced an optimized circuit for Hamming distance calculations that can be implemented on currently available quantum computing devices with high fidelity. Our circuit could act as a

mention that the data set used for this run is not related to the abstracts bag of words study, I think we need to emphasize this as reader might try to correlate those figures somehow

distance-computing component of a classical SOFMs algorithm and in this way improve its performance. Due to wide use of classical SOFMs in different areas of modern research this can give opportunities for the use of QASOFM in practical applications in near term.

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CONFLICT OF INTEREST

The authors declare no conflict of interest.

KEYWORDS

quantum self-organizing feature map; quantum machine learning; neural network; quantum unsupervised data clustering; Hamming distance.

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