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Multi-elitist immune clonal quantum clustering algorithm

Shuiping Gou *, Xiong Zhuang, Yangyang Li, Cong Xu, Licheng C. Jiao

Key Laboratory of Intelligent Perception and Image Understanding of Ministry of Education of China Institute of Intelligent Information Processing, Xidian University, Xi'an 710071, PR China

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ABSTRACT

The quantum clustering (QC) algorithm suffers from the issues of getting stuck in local extremes and computational bottleneck when handling large-size image segmentation. By embedding a potential evolution formula into affinity function calculation of multi-elitist immune clonal optimization, and updating the cluster center based on the distance matrix, the multi-elitist immune clonal quantum clustering algorithm (ME-ICQC) is proposed in this paper. In the proposed framework, elitist population is composed of the individuals with high affinity, which is considered to play dominant roles in the evolutionary process. It can help to find the global optimal solution or near-optimal solution for most tested tasks. The diversity of population can be well maintained by general subgroup evolution of ME-ICQC. These different functions are implemented by the dissimilar mutation strategies or crossover operators. The bi-group exchanges the information of excellence antibodies using the hypercube co-evolution operation. Compared with existing algorithms, the ME-ICQC achieves an improved clustering accuracy with more stable convergence, but it is not significantly better than other optimization techniques combined with QC. Also, the experimental results also show that our algorithm performs well on multi-class, parameters-sensitive and large-size datasets.

1. Introduction

Clustering analysis is an important branch of unsupervised statistical pattern recognition. Without any priori knowledge about the samples, it divides unlabeled samples into several subsets according to some criteria, so that similar samples will be grouped into the same class while dissimilar samples will be partitioned into different categories. The existing clustering algorithms include partition clustering, hierarchical clustering, density-based clustering, grid-based clustering, model-based clustering, as well as clustering technologies combined with the fuzzy theory [1], graph theory [2] and so on. The traditional clustering algorithms, like K-means clustering, have been shown to be sensitive to initialization and noise, and the number of clusters has to be predetermined [3]. Thus, the authors in [4,5] proposed a novel quantum clustering (QC) algorithm, which described the distribution of samples in the Hilbert space with a nonlinear Gaussian wave function. By solving the Schrödinger equation, the resulting potential function has the minimums which correspond to the cluster centers. The idea of QC stems from the scale-space clustering [6] and support vector clustering [7], which is essentially a type of partition nonparametric clustering technologies. Besides, QC has the advantage of discovering the inherent structures of data. It can be used in the fields of pattern recognition, bio-information mining, robot controlling and so on [8–10].

However, the classical quantum clustering algorithm has the following known drawbacks: it is quite sensitive to the selection of the scale parameter; the clustering result is prone to getting stuck in local extremes; its slow convergence has limited its application to large-size datasets. Many improved algorithms have been proposed. Zhang et al. substituted the exponent measuring distance for Euclidean distance [11]. Nasios and Bors [12] used the k-neighbor statistical distribution to estimate the kernel parameter and obtained the final partition by combining the Hessian matrix with region growing algorithm [12]. Li and Wang [13] constructed a uniform framework for QC and Fuzzy C-mean clustering algorithm (FCM) [13]. In 2009, Marvin and David explored dynamic quantum clustering methods for visual exploration of structures in data [14]. Li and Wang [13] proposed the parameter-estimated quantum clustering algorithm [15].

Some recent research has shown that the immune clonal selection algorithm [16] has the capability to find the global optimal, inspired by the biological mechanism. Compared with the existing computational intelligence methods such as genetic algorithm, Simulated annealing, and so on, immune clonal algorithm has the following advantages: the mutation operator is implemented on the memory unit but not all individual to get quickly the global optimal solution. The diversity of immune system is presented by computing the affinity to overcome the

* Corresponding author.
E-mail address: shpgou@mail.xidian.edu.cn (S. Gou).

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"prematurity" problem. Furthermore, the coevolutionary algorithm can be used to well solve high dimension numerical optimization problems [17,18]. Based on these findings, a quantum clustering algorithm with multi-elitist immune clonal optimization (ME-ICQC) is proposed in this paper. The proposed algorithm can overcome the parameter sensitivity issue and converge more quickly than QC by using immune clonal selection strategy. We divide the original population into two elite subgroups to coevolve to deal with high dimension data. In the elite subgroup, an adaptive cloud-model based mutation operator [19,20] is designed to guarantee a quick local search. General subgroup adopts a non-directional uniform hyper-mutation and all interference recombination [21] to extend the search space. After the different mutual communication of the bi-group, the multi-elitist preservation mechanism ensures the right direction of evolution. In addition, quantum potential function based simple but effective affinity formula is designed. The continuously updating of the cluster centers ensures the preferable stability and improvement in convergence speed of our algorithm. The experimental results show the computational precision and efficiency of our algorithm and its capability of dealing with large-scale dataset on public clustering and image segmentation datasets.

The remainder of this paper is organized as follows: Section 2 describes the quantum clustering algorithm. Section 3 gives the details of the proposed algorithm, including the design of algorithm, motivation analysis of population partition, as well as the geometric significance of immune operators and parameters analysis. Section 4 presents the time complexity and convergence of the algorithm. Section 5 shows the experimental results on datasets clustering together with texture image and medical image segmentation. Finally, we draw the conclusions.

2. Related work

2.1. Quantum clustering

Quantum physics estimates the locations of particles given the energy levels. Quantum clustering can be understood as the inverse of this problem. Namely, knowing the location of data samples, it calculates the states of samples under certain constraints. The quantum clustering algorithm [4,5] uses the Parzen-window method [22] and sums up all of the N data points' Gaussian (a set of basis functions) to estimate the probability distribution function $\psi(\mathbf{x})$ (for the simplicity of algebraic manipulations, in quantum mechanics the probability amplitude which determines the probability distribution is $|\psi|^2$). This can be represented as

$$\psi(\mathbf{x}) = \sum_i e^{-(\mathbf{x}-\mathbf{x}_i)^2/2\sigma^2} \tag{1}$$

where x_i is the data points and σ is the scale parameter called bandwidth or probability density estimator. $\psi(x)$is also called Gaussian wave function which assigns the ground state of Schrödinger equation and defines a map from nonlinear space to Hilbert space. According to the fifth postulate of quantum mechanics, the evolution of quantum follows the Schrödinger equation. Having known that $\psi(x)$ is one of the solutions, the time-dependent Schrödinger equation is given by

$$H\psi \equiv (-\frac{\sigma^2}{2}\nabla^2 + V(\mathbf{x}))\psi = E\psi(\mathbf{x}) \tag{2}$$

where H is the Hamiltonian operator, E is the energy eigenvalue of H, ∇^2 is the Laplacian operator, and V denotes the potential function, the minima of which determines the locations of cluster centers.

Given $\psi(\mathbf{x})$, we can solve Eq. (2) to get the general expression of potential function as

$$\begin{aligned} V(\mathbf{x}) &= E + \frac{\frac{\sigma^2}{2}\nabla^2\psi}{\psi} \\ &= E - \frac{d}{2} + \frac{1}{2\sigma^2\psi}\sum_i (\mathbf{x}-\mathbf{x}_i)^2 e^{-(\mathbf{x}-\mathbf{x}_i)^2/2\sigma^2} \end{aligned} \tag{3}$$

Let V be no-negative, that is $\min(V)=0$, E can be defined as

$$E = -\min\frac{\frac{\sigma^2}{2}\nabla^2\psi}{\psi} \tag{4}$$

Since $\psi(\mathbf{x})$is positive definite and normalized, it abstracts the data points toward minima. The Laplacian operator ∇^2 is also positive definite which diffuses the potential surface to make the data points leave the minima. They balance the effects between Laplacian's diffusion and potential function's attraction, making up of the complete distribution of particles. In the case of single point of clustering problems, it is easy to obtain $V(\mathbf{x}) = \frac{1}{2\sigma^2}(\mathbf{x}-\mathbf{x}_1)^2$. Besides, the energy eigenvalue of H is $E=d/2$ (d is the smallest possible eigenvalue of H [23], which can be the dimensionality of data samples), which is corresponding to the resonance state in quantum mechanics. This means that the ground state of potential is bounded by the single point case, it follows that:

$$0 < E \le \frac{d}{2} \tag{5}$$

Once the potential function of the initial data samples is calculated, QC uses gradient descent formula for iteration. By defining $\mathbf{y}_i(0)=\mathbf{x}_i$, where $\eta(t)$ is the iteration speed and ∇V is the gradient of potential function, the cluster center updating formula in potential minima is

$$\mathbf{y}_i(t+\Delta t) = \mathbf{y}_i(t) - \eta(t)\nabla V(\mathbf{y}_i(t)) \tag{6}$$

Then, the nearest-neighbor rule is used to obtain the partition of each cluster. The data points which are nearest in Euclidean distance with each cluster center will be partitioned into the same class. Because the scale parameter which determines the extent of diffusion on potential surface directly influences the determination of final number of cluster centers, the classical quantum clustering algorithm is quite sensitive to the scale parameter. Secondly, the speed of gradient descent method is hard to control, and the iteration is so slow. Thirdly, it is inclined to fall into local extremes by directly calculating the gradient of potential function.

2.2. Varietal quantum clustering

In order to cluster high-dimensional data, David Horn and Inon Axel proposed novel clustering algorithm for microarray expression data in a truncated SVD space [5]. Their quantum clustering method involves compression of dimensionalities achieved by applying SVD to the gene–sample matrix in microarray problems. Their quantum clustering method has one free scale parameter. Good clustering results were obtained on AML/ALL data.

Nasios et.at explored kernel-based classification using quantum mechanics [12]. They used a nonparametric estimation approach. Kernel density estimation associates a function to each data sample. The proposed approach assumes that each data sample is associated with a quantum physics particle that has a radial activation field around it. In their work, the location of each data sample is considered and their corresponding probability density function uses the analogy with the quantum potential function. The kernel scale is estimated from distributions of K-nearest neighbors statistics. This algorithm was used on