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Semi-Unsupervised Clustering Using Reinforcement Learning

Sourabh Bose and **Manfred Huber**
Department of Computer Science and Engineering
The University of Texas at Arlington
Arlington, TX USA
sourabh.bose@mavs.uta.edu huber@cse.uta.edu

Abstract

Clusters defined over a dataset by unsupervised clustering often present groupings which differ from the expected solution. This is primarily the case when some scarce knowledge of the problem exists beforehand that partially identifies desired characteristics of clusters. However conventional clustering algorithms are not defined to expect any supervision from the external world, as they are supposed to be completely unsupervised. As a result they can not benefit or effectively take into account available information about the use or properties of the clusters. In this paper we propose a reinforcement learning approach to address this problem where existing, unmodified unsupervised clustering algorithms are augmented in a way that the available sparse information is utilized to achieve more appropriate clusters. Our model works with any clustering algorithm, but the input to the algorithm, instead of being the original dataset, is a scaled version of the same, where the scaling factors are determined by the reinforcement learning algorithm.

Introduction

Clustering of data into groups is an important task to perform dimensionality reduction and to identify important properties of a data set. A wide range of algorithms for clustering have been devised that all use some built-in similarity/distance measure that is built into the algorithm to establish groupings of the data with a range of properties (Xu, Wunsch, and others 2005).These clustering algorithms group the data, attempting to maximize the distance between the clusters while minimizing the variance within the individual clusters. However, traditional clustering algorithms do not provide an efficient mechanism to fine tune the final clustering solution, given some sparse information about the desired properties of the grouping of the data.

The need of semi-unsupervised clustering arises, for example, in data sets with large numbers of attributes where most of the attributes are not semantically relevant but will dominate any distance metric (due to their number), used by traditional clustering algorithms. In these cases, sparse information regarding the quality of clusters or regarding relations between a small number of data points might be available which could be used to guide the cluster formation.

Semi-unsupervised clustering defines pairwise constraints on the input data in order to direct the clustering algorithm towards an answer which satisfies given constraints. We can have two possible types of constraints, *same cluster* or *must link constraints* which indicate that points should be in the same cluster, and *different cluster* or *must not link constraints* indicating that points should be in different clusters.

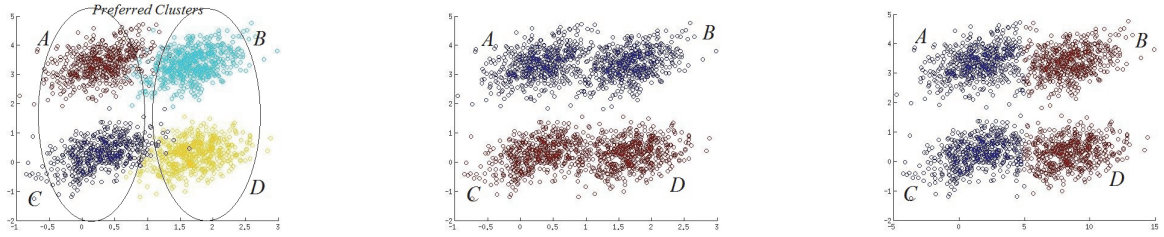
Given the input samples, it is often not possible to cluster the data according to the constraints in their original feature space using unmodified distance measures as indications for similarity. Thus we have to modify the feature space, usually by scaling the dimensions, so that an unmodified clustering algorithm is able to cluster based on it's own distance and variance constraints. In order to solve this problem, this paper presents a novel approach which, at first, learns a policy to compute the scaling factors using Reinforcement learning from a set of training problems and subsequently applies the learned policy to compute the scaling factors for new problems. The goal here is that by working on the scaled dimensions, the traditional clustering algorithm can yield results that satisfy the constraints.

Existing Methodologies

Existing methods to solve the problem usually include a regularization term in the cluster optimization criteria, therefore redefining the goal of the clustering algorithm in order to include the satisfaction of the given constraints. Using this regularization term (Zeng and Cheung 2012) these approaches modify traditional clustering algorithms (Rangapuram and Hein 2015) in order to solve for both the constraint satisfaction and the similarity optimization. The methods proposed in this area differ in the way the information is utilized either by adapting the similarity measure or by modifying the search for appropriate clusters (Grira, Crucianu, and Boujemaa 2004). Additionally, constraints often contain misleading information, which results in the miscalculation of the final cluster. To solve this problem, a subset of constraints are selected from the entire set as shown in (Zhao et al. 2012) to achieve required grouping.

Approach

Consider the set of sample data shown in Figure 1(a), generated from four distinct distributions $\{A, B, C, D\}$, which



(a) data from 4 distinct sources (b) clusters formed before scaling (c) clusters formed after scaling

Figure 1: (a): Original dataset and preferred final grouping; (b). Solution of traditional algorithm without dimension scaling; (c). Solution of the same traditional algorithm with the X-axis scaled by a factor of 5

we want to divide into two clusters. Furthermore, an additional set of constraints are posed upon the dataset, which provide evidence that the required clusters are the grouping of sets $\{A, C\}$ and $\{B, D\}$ respectively. A clustering algorithm with Cartesian distance metric applied on the data, groups the set of points into $\{A, B\}$ and $\{C, D\}$ as shown in Figure 1(b). In order for the unmodified clustering algorithm to produce the desired result, the data is scaled up along the x-axis by a factor of 5, thus increasing the distance between two points along the x-axis while keeping the y-axis variance the same. The clustering algorithm, in order to satisfy its own distance and variance optimization criteria, now additionally satisfies the point constraints, achieving the desired grouping, as shown in Figure 1(c).

For a *same cluster type* constraint, the dimensions are to be scaled in such a way that the points in the locality of the constraint pair are closer in the new feature space. This is achieved by shrinking the dimension along which they are farthest apart. Similarly for a *different cluster type* constraints the dimensions along which they are closest are expanded, pushing them farther apart in the new feature space.

If the dimensions along which scaling is performed are the same as those of the original inputs, the number and forms of the potential final clusters are limited. For example, in a two dimensional scenario the final clusters formed with two clusters can only be separated along the axes. In order to address this problem this paper presents a novel approach where the original input dimension of the dataset is appended to a kernel space with a similarity metric to each pairwise point in the set of constraints. This provides the scaling process with more degrees of freedom as it can scale along a much higher number of dimensions, resulting in a more complicated and nonlinear separation plane. Performing clustering in this reduced kernel space keeps the computational complexity lower compared to the complete kernel space over all data points. A radial basis function (RBF) is used as a kernel function (Zhang et al. 2007) since we need our kernel function to have a local property where points closer to each other should behave similarly. Thus, for input data with m samples and d dimensions we convert the data samples into a $d + 2 * c$ dimensional space where c is the number of constraints, each specifying a pair of points over which the constraint is defined. In general, this is a much smaller number than the number of samples m. For example, given a set of 10 dimensional data of 100 points and $eight$ constraints, the resultant space after conversion would be of 26 dimensions where the 10 features in the original input are concatenated with the 16 new features computed, where the similarity metric of the kernel is only computed with respect to the points in the constraints.

Upon mapping the dataset onto the new feature space, the new dimensions are scaled using a MDP (Markov Decision Process) policy learned by the Reinforcement Learning algorithm and subsequently a traditional clustering algorithm is applied on the new feature space, which now achieves the desired clusters.

Similarity Function Learning

To apply Reinforcement Learning to the learning of the effective scaling of the feature dimensions, an MDP is defined.

An MDP (Puterman 1990), $< S, A, T, R >$, defines a stochastic controllable process, where the state $s \in S$ describes all information necessary to predict the transition probabilities $T : P(S'|S, a)$ for every possible action $a \in A$. Thus policies Π defining the actions to be taken only require knowledge of the current state. The reward $R : rQ(s, a)$ defines the intermediate reward (payoff) obtained for taken action a for a given state. The goal of solving an MDP is to determine the policy $\Pi(S, a) = P(a|S)$, that maximizes the accumulated reward obtained. Reinforcement Learning is a method to learn this policy.

In this work, the MDP uses two state variables, namely, the accuracy for *same cluster* constraints and the accuracy for *different cluster* constraints. Since the variables are continuous we discretize the state space into bins of size B. It should be noted that, as with such discretizations, the choice of discretization step is a trade-off between the fine grained accuracy of the current state status and the computational complexity.

State Space of the MDP

To compute state attributes, constraints are divided into two groups, ones that are satisfied in the current clusters and ones that are not. For the ones that are not satisfied, a degree of them being satisfied is calculated. This degree is used as a

metric to identify how close to satisfied a constraint is. Using a probabilistic view on cluster membership, the probability of a point, x, being in a cluster, K_i, is defined as

$$P(K_i|x) = \frac{distance(x, K_i)}{\sum_j distance(x, K_j)}$$

The degree of a *same cluster* constraint, $C_{j,k}$, being satisfied is a function of the probabilities of the two member points, x_j and x_k, in the constraint. For each cluster, the likelihood of them lying in the same cluster, K_i, is defined as

$$P(K_i|C_{j,k}, type(C_{j,k}) = samecluster) = P(K_i|x_j) * P(K_i|x_k)$$

and the degree of a *same cluster type* constraint to be fulfilled is then calculated as the maximum product of the probabilities for each point regarding every cluster. Thus the degree of a constraint being satisfied is the maximum likelihood for any class that both points are in that cluster. The maximum (rather than the sum) is used here to achieve a stronger tie across multiple constraints containing the same data point since it forces a single cluster to be picked for each constraint. Similarly, for a *different cluster type* constraint, $C_{j,k}$, the probability of a point belonging to cluster K_i while the other does not, is defined as

$$P(K_i|C_j, k, type(C_{j,k}) = differentcluster) = P(K_i|x_j) * (1 - P(K_i|x_k))$$

and the degree of the constraint to be satisfied is again calculated as the maximum across all clusters of this probability. The accuracy of a constraint type as a state variable is defined in Equation (1).

$$P_t(satisfied) = \frac{\#satisfied\ constraints\ of\ type\ t}{\#constraints\ of\ type\ t} \quad (1)$$

$$Accuracy_t = P_t(satisfied) + (1 - P_t(satisfied)) * E_{i \in unsatisfied\ of\ type\ t}[P(K_i|C_{j,k}, type(C_{j,k}) = t)] \quad (2)$$

This results in two state attributes, $Accuracy_{same\ cluster}$ and $Accuracy_{different\ cluster}$, which are both in the range of [0..1]. We then discretize the attribute into bins of size B in order to reduce the complexity since state values closer to each other are related and thus can be grouped into a single state, the size of the group determined by the bin size B.

Action Space of the MDP

Given the degrees of satisfaction of the individual constraints of any type, the unsatisfied constraints closest to satisfaction and the constraints farthest from satisfaction are identified, i.e. for each constraint type the unsatisfied constraints with the highest and the lowest probabilities are selected. There are 4 actions which the agent can take in every state in order to satisfy the constraints.

- For *same cluster* constraint type, fix unsatisfied constraint farthest from satisfaction
- For *same cluster* constraint type, fix unsatisfied constraint closest to satisfaction
- For *different cluster* constraint type, fix unsatisfied constraint farthest from satisfaction
- For *different cluster* constraint type, fix unsatisfied constraint closest to satisfaction

Upon choosing the specific constraint to fix, the dimensions to scale are chosen. For *same cluster* constraint type, a subset of the dimensions with the highest distance is selected and scaled down, bringing them closer in the new feature space. Similarly for *different cluster* type, the dimensions with the lowest distance are selected and scaled up, pushing them farther apart.

Reward Function

The reward function is simply defined as the improvement in the satisfaction of the constraints as measured by the sum of the difference between each of the two accuracy variables of the new state and the current state.

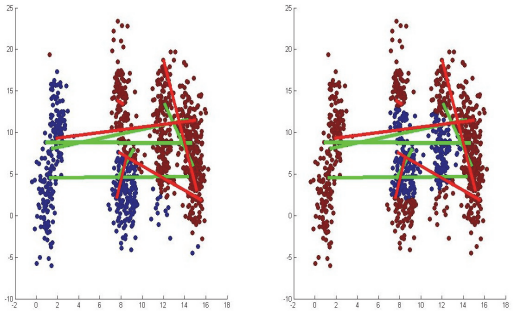
Goal State or End Criteria

The goal state is defined as the state where all the constraints are satisfied. However it is often not possible to reach this state due to many factors like human error in constraint selection or other contradicting constraints. Thus, in addition to the above goal criteria we append another condition which states that we end our search when the state does not change for a given fixed number of steps.

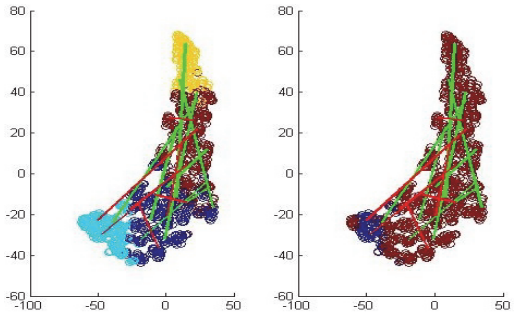
Experimental results

Problems for training, validation and testing were pseudo-randomly generated as multivariate Gaussian distributions. Parameters controlling the individual cluster size, number of distinct clusters, mean and co-variance of each cluster, along with the number of input dimensions were seeded randomly, with a range of 400 to 800 samples in each problem. Furthermore, a set of constraints for each problem were randomly chosen from the data points. Reinforcement learning was used to learn 5 different policies over a set of 70 training problems. Subsequently, the policies were used to compute the dimension scaling factors for 30 test problems similar to their respective training problems which were unseen during the policy learning phase.

For the experiments, a bin size of 0.05 was chosen, i.e. state variable values are discretized into the accuracy intervals $[0..0.05), [0.05..0.1), ..., [0.95..1]$. For the actions, scaling steps of 0.7 and 1.3 are chosen. For *same cluster* constraints the top third of the dimensions with the highest distance are scaled down by multiplying the dimensions by 0.7, and for *different cluster* constraints the bottom third dimensions are scaled up by multiplying the selected dimensions by 1.3. The algorithms used were K-means clustering (Hartigan and Wong 1979) for the clustering process and SARSA(Rummery and Niranjan 1994) as the reinforcement learning algorithm (Kaelbling, Littman, and Moore 1996) for training the MDP. The policies were trained with problems similar to each other with respect to the number of dimensions in the original dataset and the number of proposed constraints on the problem. Finally a policy was



(a) Solutions for 2-dimensional dataset



(b) Solutions for 20-dimensional dataset mapped to 2 dimensions using t-sne for visualization

Figure 2: K-means clusters. (a). Solution without dimension scaling (Left); Solution with dimension scaling (Right) (b). Solution of 20-dimensional data; Solution without dimension scaling (Left); Solution with dimension scaling (Right)

policy	# dimensions	# constraints	% satisfied
1	2 - 7	4 - 10	81.2%
2	5 - 10	20 - 25	84.8%
3	7 - 15	20 - 25	72%
4	15 - 20	10 - 15	73.33%
5	2 - 20	10 - 25	40%

Table 1: Performance analysis of individual policies

also trained with a broad range of problems, for comparison with the performance of the other specialized policies. Figure 2 shows the result of a cluster output of K-means on the original dataset and the output upon scaling the dimensions using the policies learned, red lines indicating *different cluster type* constraints while green lines indicating *same cluster type* constraints. Figure 2(a) is a solution to a 2-dimensional problem using policy 1 while, Figure 2(b) is a 20-dimensional problem, the solution to which was mapped to 2 dimensions using t-sne (Van der Maaten and Hinton 2008) for visualization. Table 1 shows the performance of the individual policies on 30 test problems and the range of dimensions and constraints learned upon. Policies $1-4$ are learned on specific types while policy 5 is a generic policy.

Since the constraints were randomly generated, it is often impossible to solve for all of them because of conflicting constraints. However, the solutions computed from the policies above solve for the highest possible number of constraints while maximizing the accuracy of unsatisfied constraints as shown in Equation (2). Table 1 also shows that policies learned for a specific type of problem (policies 1 to 4) perform much better than a generic policy (policy 5).

Conclusion

The paper shows that semi-unsupervised clustering is possible by re-mapping and scaling the original input dimensions, without modifying the clustering algorithm. Thus, this method can be applied to any traditional clustering algorithm. This paper also shows that performance of generic is poor compared to policies from specific types of problems.

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