Evolutionary star-structured heterogeneous data co-clustering

Amit Salunke

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Evolutionary Star-Structured Heterogeneous Data Co-Clustering

by

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A Thesis Submitted in Partial Fulfillment of the Requirements for the Degree of Master of Science in Computer Science

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Abstract

A star-structured interrelationship, which is a more common type in real world data, has a central object connected to the other types of objects. One of the key challenges in evolutionary clustering is integration of historical data in current data. Traditionally, smoothness in data transition over a period of time is achieved by means of cost functions defined over historical and current data. These functions provide a tunable tolerance for shifts of current data accounting instance to all historical information for corresponding instance. Once historical data is integrated into current data using cost functions, co-clustering is obtained using various co-clustering algorithms like spectral clustering, non-negative matrix factorization, and information theory based clustering. Non-negative matrix factorization has been proven efficient and scalable for large data and is less memory intensive compared to other approaches. Non-negative matrix factorization tri-factorizes original data matrix into row indicator matrix, column indicator matrix, and a matrix that provides correlation between the row and column clusters. However, challenges in clustering evolving heterogeneous data have never been addressed. In this thesis, I propose a new algorithm for clustering a specific case of this problem, viz. the star-structured heterogeneous data. The proposed algorithm will provide cost functions to integrate historical star-structured heterogeneous data into current data. Then I will use non-negative matrix factorization to cluster each time-step of instances and features. This contribution to the field will provide an avenue for further development of higher order evolutionary co-clustering algorithms.
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1. Introduction

Rapid development in data acquisition technology has resulted in the generation of large amounts of raw data, providing significant potential for the development of automatic data retrieval, analysis and mining. Data clustering is a well-known and widely used data mining technique that groups data objects into different groups (known as clusters) based on a predefined criterion of similarity [19] [20]. In other words, objects in a cluster are similar to each other, while being dissimilar from the ones in a different cluster. Traditional clustering methods perform one dimensional clustering, i.e. clustering of instances alone, and fail to extract any information from the features [42].

Data co-clustering not only clusters instances and features together, but also extracts relationships between instances and features being clustered [2] [10] [11] [13]. In general, co-clustering problems involve two types of data that are pair-wise heterogenous in nature and need to be clustered together. Dhillon [10] modeled the problem of co-clustering as a graph partitioning problem. He performed co-clustering on words and documents dataset using an singular value decomposition based algorithm to partition a bipartite graph between word-document. Rege et al. [29] proposed an isoperimetric co-clustering algorithm that is again a bipartite partitioning-based co-clustering model. Recently, it has been shown that Non-negative Matrix Factorization (NMF) algorithms are less memory intensive and outperform graph-based methods like spectral co-clustering (SVD) and iso-perimetric co-clustering (ICA) in achieving higher accuracy and efficiency [24] [40] [7] [33].

In the real world, data types in domains such as multimedia [4], biomedicine [12] [28] [41], and web mining [30] [39] are multi-type in nature. For example, Web images that are generally surrounded by text describing the image can be clustered using their low-level features like color and texture or surrounding text describing the images [43] [37] [15] [31]. However, pairwise co-clustering extracts the pair-wise relation in bi-type data like
words and documents but fails to extract relations in higher-order heterogeneous data like Web images. Rege et al. (CIHC) [31] and Gao et al. (CBGC) [15] modeled such problems of heterogeneous data co-clustering as tripartite graph partitioning problems. Long et al. [23] proposed a spectral clustering-based approach for higher-order heterogeneous data co-clustering. Recently, non-negative matrix factorization has been used in order to perform heterogeneous data co-clustering [7].

However, all of these efforts have been limited to static data. Data extracted from certain domains like social networks and web-blogs are evolving in nature. In these domains, data collected over a short time interval exhibit high similarity over data instances and features. This can be effectively used to optimize data clustering since changes in clustering are gradual [6]. None of the algorithms discussed above take into account the passage of time and knowledge that can be gained by observing data as it evolves. Chakrabarti et al. [6] and Chi et al. [8] have shown that incorporation of historic knowledge improves the clustering accuracy. Wang et al. [38] proposed that evolutionary clustering can be effectively done by the amalgamation of low-rank matrix approximation methods and matrix factorization-based clustering. Recently, Green et al. [16] proposed an evolutionary spectral co-clustering approach for evolutionary data.

In the case of data extracted from domains like social networks and web blogs, the data is heterogeneous as well as evolutionary. In spite of efforts on heterogeneous co-clustering and evolutionary co-clustering algorithms, the problem of co-clustering-evolving-heterogeneous data has not been addressed. To the best of my knowledge, there are no contributions toward an algorithm that performs co-clustering on evolving heterogeneous data. In this thesis, I propose a novel algorithm designed for co-clustering of evolving heterogeneous data. The proposed algorithm is entitled EHCC (Evolutionary star-structured Heterogeneous Co-Clustering), which will perform non-negative matrix factorization over multiple time slices to handle evolving data. In order to perform co-clustering on evolutionary heterogeneous data, the current data is augmented by incorporating historical information by using a cost function [6] [8] [16]. Non-negative matrix factorization is then performed to
obtain the desired co-clustering results for the star-structured evolutionary data [7].

The rest of the thesis is organized as follows. Chapter 2 discusses several representative backgrounds and related work. Chapter 3 presents the proposed Evolutionary star-structured Heterogeneous Co-Clustering method, the core algorithm of this thesis, in detail. Experiments and results appear in Chapter 4. Finally, Chapter 5 concludes the thesis and discusses the future work.
2. Background and Related Work

In this chapter, I provide a review of related work. First I introduce Evolutionary Clustering/Co-clustering. Then I briefly describe Star-Structured Heterogeneous Data Co-Clustering algorithms in the literature. The chapter end with an overview of Low-rank Matrix Approximation.

2.1 Evolutionary Clustering/Co-clustering

Chakrabarti et al. [6] were among the first few to introduce the concept of evolutionary clustering. They proposed evolutionary versions for widely used clustering algorithms, viz., k-means and hierarchical clustering. They considered evolutionary clustering as an optimization problem between two contrasting criteria; the first is that clustering should reflect current data clustering, and the other is that, at any point in time, data clustering should not differ drastically from previous time-step data. They presented current cost as trade off between historic data and current data. The goal of the evolutionary clustering algorithm is to minimize the overall cost - keeping the historic cost to a minimum (keeping current data clustering similar to the previous clustering in the sequence) and current cost to a maximum (providing high-quality current clustering of the data). Chakrabarti et al. perform evolutionary k-means by integrating historic data in current data as follows 2.1.

\[ J_{cost} = -\alpha \cdot f_{sq} + (1 - \alpha) \cdot f_{hc} \] (2.1)

In equation 2.1, \( \alpha \) is tradeoff between historic data (historic quality) and current data (snapshot quality), and \( 0 \leq \alpha \leq 1 \).
In [8], Chi et al. make use of the spectral clustering algorithm to extend evolutionary clustering introduced in [6] by adding temporal smoothing through two evolutionary frameworks. The first framework, preserving cluster quality (PCQ), was designed to measure how well clusters appropriately accounted for historical data. The second framework, preserving cluster membership (PCM), was designed to measure the difference between the current clustering and the next previous clustering. In either case these measures were the temporal cost of the current cluster choices. The temporal cost weighed into the quality of the partitions. Authors define temporal smoothness as how effective clustering results on data at current time step with respect to clustering results on historical data. The framework makes use of same cost function used by Chakrabarti et al. [6]. They defined cost function for PCQ (measuring how well clusters appropriately accounted for historical data) as,

\[
\text{Cost}_{NC} = k - Tr[X_t^T \left( \alpha D_t^{-\frac{1}{2}} W_t D_t^{-\frac{1}{2}} - (1 - \alpha) D_{t-1}^{-\frac{1}{2}} W_{t-1} D_{t-1}^{-\frac{1}{2}} \right) X_t]
\]

where \(t\) refers to the current time step, \(W \in \mathbb{R}^{n \times m}\) is bi-type relational data, \(D\) is the diagonal singular matrix for the relational data \(W\), \(k\) is number of clusters, \(X\) is a construct, and \(Tr()\) is a trace function.

Green et al. [16] extend the approach presented in [8] to spectral co-clustering. They introduced evolutionary co-clustering. The proposed two approaches, Respect To the Current (RTC) and Respect To Historical (RTH), perform co-clustering on evolving instances as well as features. The construct \(X_t\), represents an evolutionary clustering for the bi-type relational data with RTC as,

\[
X_t = \text{svd}[\alpha W - (1 - \alpha) D_{t-1}^{-\frac{1}{2}} W_{t-1} D_{t-1}^{-\frac{1}{2}}]
\]

Recently, Wang et al. [38] proposed a kernel matrix-based evolutionary clustering algorithm for large-scale evolutionary data. Amalgamation of low-rank approximation to the clustering algorithm reduces original large data into non-redundant subspace without
compromising the accuracy of the clustering algorithm. They also propose clustering using non-negative matrix factorization, which is more scalable for large data and is more accurate and efficient compared to other clustering approaches like spectral clustering.

### 2.2 Star-Structured Heterogeneous Data Co-Clustering

In the case of a Star-Structured Heterogeneous Data, a central data object is connected to other types to form a star structure of the interrelationships as shown in Figure 2.1. Gao et al. [15] proposed Consistent Bipartite Graph Co-clustering (CBGC) for clustering this kind of data. Long et al. [24] proposed a spectral-clustering-based approach for multi-type relational data that generalized the approach for higher-order heterogeneous data co-clustering. In [31] [25], Rege et al. proposed the Consistent Isoperimetric High-order Co-clustering (CIHC) framework for partitioning the star-structured graphs. The proposed algorithm partitions fusion of bipartite graphs. The algorithm is quick since it obtains a solution to a sparse system by solving linear equation simultaneously. Long et al. [23] formulated heterogeneous co-clustering as collective factorization on related matrices and obtained co-clustering by deriving sub-matrices by simultaneously clustering multi-type interrelated data. This algorithm provides more flexibility toward heterogeneous co-clustering since the framework is applicable for general case data interrelationship. Graph-partitioned-based co-clustering methods produce negative values in spite of the original data matrix.
being positive. This can be difficult to interpret for applications like documents and image clustering since they always have positive input. Matrix-factorization-based clustering approaches have received increased attention due to their applicability to high dimensional datasets. Chen et al. [7] proposed non-negative matrix factorization for heterogeneous data co-clustering. They performed trifactorization using an iterative algorithm to obtain new cluster indicator matrices and the correlation between interrelated data. They show that non-negative factorization outperforms graph-based methods and is less memory intensive. Hence, they are efficient and scalable for large data.

2.3 Low-rank Matrix Approximation

Low-rank approximation methods extract correlation and then remove redundancy from data to obtain sparse data [1]. One way to make clustering algorithms computationally efficient is to integrate a data mining algorithm with low-rank approximation methods. Singular Value Decomposition (SVD) is widely used for low-rank approximation since it optimally calculates approximation using the Frobenius norm. However, SVD does not produce a sparse matrix that is computationally very effective. Berry et al. [3] proposed an improved low-rank approximation approach (Algorithm 844) called quasi-Gram-Schmidt-algorithm based on the classical Gram-Schmidt algorithm. They trifactorized the input matrix into two full-rank matrices and a non-singular matrix that is more efficient in terms of computational power and space storage than SVD. Petros et al. [14] aims to address the problem of memory access time (seek-time) for a large data set using the family of CUR algorithms, namely LINEARTIMECUR and CONSTANTTIMECUR, based on fast Monte Carlo algorithms. The LINEARTIMECUR algorithm makes use of the original data matrix with two passes over existing storage of the matrix in external memory without storing on RAM. The other algorithm, CONSTANTTIMECUR, focuses on optimization of seek time. The advantage of the CONSTANTTIMECUR algorithm approach over the LINEARTIMECUR algorithm is the CONSTANTTIMECUR algorithm does not require additional RAM;
however, it requires additional pass-over main memory, and the new low-rank approximation matrix has an additional error. SVD and CUR are capable of identifying the correlation and hidden structure in a data set, but they are not efficient enough to obtain computationally efficient sparse matrix. Sun et al. [34] addressed this problem by proposing a new approximation method, the Compact Matrix Decomposition (CMD), which focuses on reducing the high memory usage and computational cost for large sparse graphs. The authors express the association between two nodes of a graph using the relational matrix such that every element represents the degree of similarity between two nodes of the object. They removed the redundancy of nodes by sampling and removing the null row or column entries and projecting original data into new subspace. Pan et al. [27] proposed a framework (CRD) that achieves a linear-time low-rank approximation by utilizing sampling-based matrix decomposition methods and perform partition-based co-clustering on large data. The proposed framework decomposed the original data matrix into subsets of rows and columns and performs co-clustering using matrix decomposition using an approach like block-value decomposition [24]. Since subspace is created using random sampling, re-sampling is needed to avoid a case where the entire cluster is not sampled while random sampling. Chebyshevs Inequality was used to detect such rows and columns and reduce the error rate because of biased sampling. Low-rank algorithms like CUR and CMD focused on preserving sparsity in large-graph data by creating a smaller subspace to represent original data by sampling it. However, they were overly complicated and were not able to optimize the sub-space calculation either with time or space. To address these issues, Tong et al. [36] proposed two algorithms, Colibri-S and Colibri-D, for static and dynamic graphs, respectively. They proposed solution in which they first performed bias sampling by creating an initial subspace that consisted of linearly dependent columns or near duplicates. Then they optimized subspace by iterative sampling and removing all dependent columns or duplicates. The authors showed that proposed algorithms for static and dynamic graphs are very efficient.
3. Evolutionary Star-Structured Heterogeneous Data Co-Clustering

In this chapter, I present an evolutionary star-structured heterogeneous data co-clustering algorithm. Specifically, I will discuss 1) how to incorporate historical data into current data and 2) how to efficiently infer clusters of different data types simultaneously using non-negative matrix factorization (NMF).

3.1 Evolutionary Star-Structured Heterogeneous Data

In the case of a Star-Structured Heterogeneous Data at a time step $t$, we represent multi-type relational data of $m$-types using relational matrices with central data type $c$ connected to $p$ other data types. The relation between every data type with central data type is represented using relational matrix $W_t^{(ci)} \in \mathbb{R}^{n_c \times n_i}$. For example in Figure 3.1, central data $c$ is connected to four other data types, and we represent their relationship with central data type using relational matrices $W_t^{(c1)}$, $W_t^{(c2)}$, $W_t^{(c3)}$, and $W_t^{(c4)}$, respectively.

3.2 Data dynamics and Low-rank Matrix Approximation

One of the challenges of evolutionary data is the dynamic nature of the data. Over a period of time, we have changes in data size (changes in number of samples and features of data) as well as changes in the structure of data (changes in number of clusters in the data). Low-rank approximation methods extract correlation and then remove redundancy from data to obtain sparse data. This makes the original data mining algorithm computationally efficient on large data sets.
Figure 3.1: The Star-Structured Heterogeneous Data.

The family of Colibri methods [36], i.e., Colibri-S (Low-rank approximation method for static data) and Colibri-D (Low-rank approximation for dynamic data), has proven more efficient in terms of space and time compared to others like CRD [27], CMD [34], and CUR [14]. Specifically, for dynamic data there is a gradual change in data between two consecutive time steps. Colibri-D takes leverage of the similarity between two consecutive time steps to quickly update the approximating subspace. To integrate historic data into current data, we make use of Colibri-D to obtain approximating historic subspace compatible with respect to current data. First, we use the Colibri-S algorithm to calculate initial biased subspace [36]. Colibri-S iteratively constructs optimized subspace by eliminating redundant columns. In the first stage, we simply follow the CUR [14] algorithm to sample a small subset of columns from the data matrix with replacement, biased toward those with higher norms. Then we initialize the output matrix with the first column of the data matrix and then iteratively select a new column from biased subspace, which is linearly dependent on the current columns. We finally obtain a matrix by removing all the redundant columns. Colibri-D makes use of subspace calculated at time $t$ to calculate subspace at time $t-1$. Since the change in graph between two consecutive time steps is assumed to be reasonably small, the overall edges affected between two time steps are far too less. Hence, for dynamic data, once we obtain initial subspace using Colibri-S, then we update subspace for modified data.
a over period of time. So, authors have proposed a faster method to update output matrix by sampling and comparing sampled edges between two time steps \( t \) and \( t-1 \). The output thus obtained is compatible with respect to current data and is computationally efficient.

Before we apply low-rank approximation using the Colibri family to obtain sparse compatible historical data with respect to current data, we make sure the dimension of historical data is larger than current data, so that when we apply Colibri-D, we get data dimensions of historical data equal to that of current data. In the case where historical data has less number of instances and/or features, we determine differences in instances and/or features between historical data and current data, and we add those instances and/or features into the historical data matrix. The inserted instance or feature receives the average of the whole matrix at the current time step for each cell. We then apply Low-rank approximation to project original data \( W_t(\cdot) \in \mathbb{R}^{n_c \times n_t} \) into subspace \( \widehat{W}_t(\cdot) \in \mathbb{R}^{n_c \times n_t} \) to improve computational efficiency of the algorithm in both time and space: clustering accuracy remains unaffected.

We define the overall cost function of EHCC (Evolutionary star-structured Heterogeneous Co-Clustering) as the sum of snapshot quality and historical cost. We solve this problem by maximizing the clustering quality of the current snapshot and minimizing the historical cost that provides clustering smoothness [6] [8] [38]. We propose an optimization equation to obtain EHCC for evolutionary higher-order relational data matrix \( \widehat{W}_t(\cdot) \in \mathbb{R}^{n_c \times n_t} \) and \( t = (t, t-1) \) as,

\[
J = \min_{L^{(c)}_t, M^{(c)}_t, R^{(i)}_t} \left[ \sum_{(c)} \alpha \cdot \| \widehat{W}_t(\cdot) - L^{(c)}_t M^{(c)}_t R^{(i)}_t \|^2 
+ (1 - \alpha) \cdot \| \widehat{W}_{t-1}(\cdot) - L^{(c)}_{t-1} M^{(c)}_{t-1} R^{(i)}_{t-1} \|^2 \right] \quad (3.1)
\]

where \( \alpha \) is a trade off between historic data (historic quality) and current data (snapshot quality), and \( 0 \leq \alpha \leq 1 \). \( L^{(c)}_t \in \mathbb{R}^{n_c \times k_c} \) (row coefficient matrix) and \( R^{(i)}_t \in \mathbb{R}^{k_i \times n_i} \) (column coefficient matrix) are indicator matrices representing soft-clustering for instances and features, respectively, and \( M^{(c)}_t \in \mathbb{R}^{k_c \times n_i} \) (block value matrix) is the co-relation indicator matrix.
that represents the co-clustering relation between central data type and each data type con-
nected with central data type at time step $t$ [24] [40] [7].

We generalize the optimization equation (3.1) for multiple time step data represented
by, $\tilde{W}_{t}^{(ci)} \in \mathbb{R}^{n_c \times n_i}$ for $t=\{1, 2, ..., S\}$, where is $S$ last time-step in data,

$$J = \min_{L_t^{(c)}, M_t^{(c)}, R_t^{(i)}} \sum_{t=1}^{S} \alpha (1 - \alpha)^{S-t} \cdot \|	ilde{W}_{t}^{(ci)} - L_t^{(c)} M_t^{(ci)} R_t^{(i)} \|^2$$ \hspace{1cm} (3.2)

### 3.3 Estimating the Number of Clusters

In unsupervised learning methods, automatic estimation of number of clusters in data is
a challenging task [20]. For evolutionary data, the shape of data changes over a period
of time. We have change in the number of clusters over a period of time. For automatic
cluster estimation, we use six different well-known methods for cluster estimation, namely,
Silhouettes [32], Davies-Bouldin index [9], Calinski-Harabasz index [5], Krzanowski-Lai
index [21], and Hartigan [17] and weighted inter-to intra-cluster ratio with Homogeneity
and Separation index [35]. Because that data is gradually evolving, we make use of cluster
estimation on historical data to estimate the number of clusters in current data. The process
is faster since we need to estimate the number of clusters closer to the previously estimated
value only. We estimate the number of clusters using previously mentioned methods and
use the mode from the above estimation methods to decide the number of clusters in current
data.

### 3.4 Co-clustering using Non-negative Matrix Factorization

Since non-negative matrix-factorization-based co-clustering methods have been more ef-
ficient than graph-based methods in terms of efficiency and accuracy for large data sets
like document and image clustering, and they are easy to interpret, we use a non-negative
factorization-based method to obtain co-clustering. The minimization of (3.2) can be
achieved by updating one factor while keeping the others constant. We solve the above
optimization problem (3.2) through following the iterative solution to obtain $L_S^{(c)}$, $R_S^{(i)}$ and $M_S^{(c_i)}$ [38]. This iterative process seeks to minimize equation as rules specified in algorithm 1.
Algorithm 1 Evolutionary Star-Structured Heterogeneous Data Co-Clustering

**Input:** A relational matrix $W_t^{(ci)} \in \mathbb{R}^{n_{ci} \times n_t}$ for $t=\{1, 2, \ldots, S\}$

**Output:** $L_t^{(ci)} \in \mathbb{R}^{n_{ci} \times k_c}$ (row cluster indicator matrix) and $R_t^{(i)} \in \mathbb{R}^{k_i \times n_t}$ (column cluster indicator matrix) and $M_t^{(ci)} \in \mathbb{R}^{k_c \times k_i}$ (block value matrix)

1: for $t \leftarrow 2, S$ do
2: \hspace{1em} for $i \leftarrow 1, p$ do \{If time-step $W_{t-1}^{(ci)}$ has less number of instances than $W_t^{(ci)}$, add new instances to $W_{t-1}^{(ci)}$\}
3: \hspace{2em} if $\text{lengthof}(W_{t-1}^{(ci)}) < \text{lengthof}(W_t^{(ci)})$ then
4: \hspace{3em} for $j \leftarrow \text{lengthof}(W_{t-1}^{(ci)}), \text{lengthof}(W_t^{(ci)})$ do
5: \hspace{4em} insert $\mu(W_t)$
6: \hspace{4em} add instance insert to $W_{t-1}^{(ci)}$
7: \hspace{2em} end for
8: \hspace{1em} end if
9: \hspace{1em} \{If time-step $W_{t-1}^{(ci)}$ has more number of instances than $W_t^{(ci)}$, add new instances to $W_{t-1}^{(ci)}$\}
10: \hspace{1em} if $\text{lengthof}(W_{t-1}^{(ci)}) > \text{lengthof}(W_t^{(ci)})$ then
11: \hspace{2em} Use intermediate results from the Colibri method to get unique and independent subspace from $W_{t-1}^{(ci)}$ equivalent to length of $W_t^{(ci)}$
12: \hspace{1em} end if
13: \hspace{1em} \{If time-step $W_{t-1}^{(ci)}$ has fewer features than $W_t^{(ci)}$, add new instances to $W_{t-1}^{(ci)}$\}
14: \hspace{1em} if $\text{featurelengthof}(W_{t-1}^{(ci)}) < \text{featurelengthof}(W_t^{(ci)})$ then
15: \hspace{2em} for $j \leftarrow \text{featurelengthof}(W_{t-1}^{(ci)}), \text{featurelengthof}(W_t^{(ci)})$ do
16: \hspace{3em} insert $\mu(W_t^{(ci)})$
17: \hspace{3em} add feature insert to $W_{t-1}^{(ci)}$
18: \hspace{2em} end for
19: \hspace{1em} end if
18: \textbf{if} featurelengthof(W^{(ci)}_{t-1}) > featurelengthof(W^{(ci)}_t) \textbf{then} //If time-step 
19: \hspace{1em} W_{t-1} has more features than W_t, add new instances to W_{t-1} \} 
end if
20: Use intermediate results from the Colibri method to get unique and independent subspace from W^{(ci)}_{t-1} equivalent to feature length of W^{(ci)}_t 
\{ //Use the Colibri-D method to obtain Low-rank approximation of W_{t-1} with 
21: \text{TEMPW}^{(ci)}_t \leftarrow Colibri - D(W^{(ci)}_{t-1}, W^{(ci)}_t) 
22: \text{W}^{(ci)}_t \leftarrow \alpha \cdot W^{(ci)}_t + (1 - \alpha) \cdot \text{TEMPW}^{(ci)}_t 
end for
24: end for
25: Estimate number of cluster in \text{W}^{(ci)}_t using methods mentioned in section 3.3.
26: Obtain clustering using the following rules by applying recursive on \text{W}^{(ci)}_t
\begin{equation}
L^{(c)}_{(S)(ab)} \leftarrow L^{(c)}_{(S)(ab)} \frac{\sum_{i=1}^{p} ((\sum_{i=1}^{S} \alpha(1 - \alpha)^{S-t} \cdot \text{W}^{(ci)}_t)R^{(i)}_{(S)} M^{(ci)(a)}_{(S)} )_{ab}}{\sum_{i=1}^{p} (L^{(c)}_{(S)} M^{(ci)}_{(S)} )_{ab}
(3.3)
\end{equation}
\begin{equation}
R^{(i)}_{(S)(ab)} \leftarrow R^{(i)}_{(S)(ab)} \frac{(M^{(ci)(a)}_{(S)} L^{(c)}_{(S)} )_{ab}}{(M^{(ci)(a)}_{(S)} L^{(c)}_{(S)} )_{ab}}
(3.4)
\end{equation}
\begin{equation}
M^{(ci)}_{(S)(ab)} \leftarrow M^{(ci)}_{(S)(ab)} \frac{(L^{(c)}_{(S)} )_{ab}}{(L^{(c)}_{(S)} )_{ab}}
(3.5)
\end{equation}
subject to the constraints \forall_{ab}: L^{(c)}_{S(ab)} \geq 0 \text{ and } R^{(i)}_{S(ab)} \geq 0, \text{ where } ||.|| \text{ denote Frobenius matrix norm, } L^{(c)}_S \in \mathbb{R}^{n \times k}, M^{(ci)}_S \in \mathbb{R}^{k \times l}, R^{(i)}_S \in \mathbb{R}^{l \times m}, k \ll n, \text{ and } l \ll m.
4. Experiments

In this chapter, we demonstrate the performance of EHCC. We evaluated proposed algorithm on variety of datasets, synthetic as well as real world datasets. Section 4.1 describes datasets and preprocessing information. In section 4.2, we describe experiment evaluation method. Finally, in section 4.3, we explain experiment and results.

4.1 Data Description and Preprocessing

We performed two sets of experiments to determine validity of proposed algorithm. We run first set of experiments on a synthetic dataset, generated to evaluate different proposed functionalities of the algorithm. For the second set, we used real world datasets from three different domains, viz. web-service data, publicly available text-datasets, and image dataset.

4.1.1 Synthetic Data

We performed two different experiments on synthetic data to test different features of proposed algorithm. The first experiment demonstrates the ability of the algorithm to handle instance and/or feature evolution, addition of instances and/or features, removal of instances and/or features as well as the consistency across similar time-steps. The second experiment shows algorithm’s ability to handle cluster shift over period of time. The experiment tests instance as well as feature drift.

We generated a synthetic dataset consisting 8 time-steps, with step having 5 clusters of 200 instances. For initial time-step, the 5 clusters were generated from 5 normal distributions. Every cluster was distanced from each other through an augmented $\mu$ value. So, for
each cluster $C_n$, the distribution is determined by equation, $\mu_n = \mu_{n-1} + 5 \cdot n + R$, where $R$ is an integer randomly selected from [0-100]. For all distribution, standard deviation, $\sigma$ is equal to 1.

### 4.1.2 Web-Service Community Formation

A WSDL document consists of five key components: types, messages, portType, binding, and service. Inspired by information retrieval techniques [26], we model services and operations as vectors of functional terms as these terms represent the functionalities that the services or operations provide. We apply traditional data processing techniques, which involve extraction, tokenization, stopword removal and stemming, to obtain the functional terms from the five WSDL components. Extraction identifies the key terms in a WSDL document. Since terms in WSDL documents are usually stored in composite format (e.g., groceryStoreFood), tokenization is used to derive simple terms (e.g., grocery, store, food). Non-functional terms and WSDL specific keywords such as http, url, host are removed by the means of stopword removal. Finally, stemming is applied to reduce different forms of a term into a common root (e.g. write, writing, and wrote get reduced to write). After data processing is completed, each service and operation will be represented as a vector of their respective functional terms. Using these vectors, we construct a *term-by-service* matrix and an *operation-by-term* matrix. The dataset represents a tri-type data environment with *terms* as the central data type. The *terms-operations* matrix consists of 384 terms and 72 operations. In the *term-by-service* matrix we have 384 terms and 97 services. Terms are collected by processing WSDL files from 5 different domains, namely, Communication, Education, Food, Medical and Travel. So, every data type has 5 clusters.

### 4.1.3 Text Co-clustering

In this section, we evaluate our proposed algorithm for *word-document* co-clustering by using four datasets from different sources. We used data sets oh0,oh5, oh10 and oh15 from
OHSUMED collection [18]. Data set re0 is subset of the Reuters-21578 text categorization dataset [22]. We mix these datasets as below.

- Dataset *England-Heart* was created by mixing classes *England* and *Heart-Valve-Prosthesis* from *oh0* dataset.

- Classes *Graft-Survival* and *Phospholipids* from *oh5* were mixed to form the *Graft-Phos* dataset.

- *ArachidonicAcids-Hematocrit* was derived from *oh10* using *Arachidonic Acids* and *Hematocrit* classes.

- *Enzyme Activation* and *Staphylococcal Infections* were mixed to obtain the *Enzyme-Infections* dataset.

To analyze performance of the algorithm, we compared our results with [7] [13] [24]. We performed feature selection to select top 1,000 words. We construct document-category matrix by calculating the probability of each document belonging to each category. For each document, if any of the top 1,000 word occurs, then we considered word occurrence 1 else 0. Then, we calculated probability of one document belonging to a category as the ratio of the sum of occurrence of selected top 1,000 words in this document to 1,000. We mix dataset from OHSUMED collection with *re0* to form higher-order dataset. Tables 4.1 gives the details of datasets we used.

Table 4.1: Data sets for (word-document-category) co-clustering

<table>
<thead>
<tr>
<th>Data Set</th>
<th>No. of Documents</th>
<th>No. of Categories</th>
<th>No. of Document clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>England-Heart, re0</em></td>
<td>913</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td><em>Graft-Phos, re0</em></td>
<td>831</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td><em>ArachidonicAcids-Hematocrit, re0</em></td>
<td>812</td>
<td>2</td>
<td>4</td>
</tr>
<tr>
<td><em>Enzyme-Infections, re0</em></td>
<td>849</td>
<td>2</td>
<td>4</td>
</tr>
</tbody>
</table>

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4.1.4 Image Co-clustering

For our experiments on image datasets, we chose images from Corel-CDs which contains general-purpose images from different domains such as automobiles, landscape, animal, automobiles, etc. For image co-clustering, we represented each image in the form of vector of 45 color features, 42 texture features [43] [37]. 45 color features consist of color channels(RGB, 9 features, including mean, variance, and skewness of R, G, and B channels), color coherence vector(CCV, 24 features), and color histogram (CH, 12 features). Gabor wavelet based texture (Gab, 24 features), edge direction histogram (EDH, 9 features), and edge direction coherence vector (EDCV, 9 features) were extracted from each image to represent image using Texture features. We constructed two matrices, image-color and image-texture representing color and textures features respectively.

We selected 500 images from 5 different contents, namely, African Lion, African Elephant, sunsets, bonsai, and aviation. Some examples from each category are shown in Figure 4.1. In the proposed relevance feedback framework, we collect the users’ positive feedback as samples to construct image-log matrix. Through feedback, the images marked indicate that they are similar to each other according to user’s preference also called as a log. In every log, user marks 3-5 similar images from 20 images randomly selected from image pool. We mark similar images by 1 for rest images in log-images vector we mark 0 to obtain image-log matrix.
4.2 Evaluation Method

We calculate clustering accuracy using micro-averaged precision value, given by,

\[ AC = \frac{\sum_{i=1}^{n} \Phi(X_i, Y_i)}{n} \]  

where \( n \) is number of instances in central data type, \( \Phi(X_i, Y_i) \) is equal to 1 if assigned label \( Y_i \) and true label \( X_i \) for instance \( i \) is same, else it is 0. Since the algorithm is solved by iterative solution, it does not guarantee to find the global minimum. So we ran each
We evaluated performance of evolutionary algorithm by comparing its performance against individual clustering at a time-step $t$ without considering historic data.

4.3 Experiment Results

4.3.1 Synthetic Data

At time-step $t_1$, Gaussian noise of 50 instances was added per cluster. At time-step $t_2$ 10 more instances were added from distribution of $C_2$. At time-step $t_3$ 10 instances were removed from cluster $C_4$. At time-step $t_4$, 2 features were added to $C_4$. 1 feature was removed from $C_1$ at time-step $t_5$. $t_7$ is unchanged from $t_6$. Figure 4.2 shows visualization of data over period of time from $t_0$ to $t_7$. In Figure 4.3, we show evolutionary higher order clustering out performs higher order clustering. As proposed, the algorithm is capable of handling data dynamics over period of time. At time-step $t_1$, despite of adding Gaussian noise, clustering at $t_1$, is almost unchanged. At time-steps $t_2$ additional instances from same distribution of clusters were added to dataset, and algorithm is capable of appropriately clustering them. Similarly, at $t_3$, we removed 10 instances from a cluster, and algorithm produced stable results opposing the process of removal of instance over period of time. At $t_4$, data as well clustering remained unchanged, indicating stability of the algorithm when data is unchanged. At time-step $t_5$, the algorithm has clustered added features $C_4$. Even though the accuracy of algorithm slightly decreased, however, it has performed well than static higher order co-clustering. Similarly, when we removed feature from dataset, algorithm has shown resistance to the change in clustering at time-step $t_6$. Clustering at $t_7$ again shows stability of algorithm when data is unchanged.
Figure 4.2: Visualization of Synthetic data clustering over period of time from $t_0$ to $t_7$: At time-step $t_1$, Gaussian noise of 50 instances was added per cluster. At time-step $t_2$ 10 more instances were added from distribution of $C_2$. At time-step $t_3$ 10 instances were removed from cluster $C_4$. At time-step $t_5$, 2 features were added to $C_4$. 1 feature was removed from $C_1$ at time-step $t_6$. $t_7$ is unchanged from $t_6$. 

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To evaluate algorithm’s ability to handle instance drift, we augmented original dataset. We chose and modified of 20 instances from cluster $C_4$. At each time-step, we progressively modified the distribution of those instances towards $C_5$ so that at time step $t_7$ those instances originally from $C_4$ have same distribution as those in $C_5$. In other words, we progressively moved them from $C_4$ to $C_5$ over period of time. From Figure 4.4 shows clustering of data over period of time. We show instances are progressively drifted from $C_4$ to $C_5$ over period of time.
Figure 4.4: Visualization of Synthetic data clustering over period of time from $t_0$ to $t_7$; $t_0$ is the original data. Between time steps $t_1$ - $t_6$, instances shown drift from $C_4$ to $C_5$. Finally, at time step $t_7$, 20 instances moved from $C_4$ to $C_5$.

To evaluate algorithm’s ability to handle feature drift, we augmented original dataset. We chose and modified of 2 features from cluster $C_4$. At each time-step, we progressively modified the distribution of those features towards new cluster $C_6$ so that at time step $t_7$ those features originally from $C_4$ have same but new distribution from that of $C_5$. In other
words, we progressively moved them from $C_4$ to $C_6$ over period of time. A new cluster started appearing at $t_4$. At $t_5$ both features moved to same cluster to form $C_6$. Over next few time steps, cluster has become more homogeneous. Figure 4.5 illustrate our observations.

Figure 4.5: Visualization of Synthetic data clustering over period of time from $t_0$ to $t_7$ : $t_0$ is the original data. Between time steps $t_1$ - $t_6$, features shown drift from $C_4$ to new cluster $C_6$. At time step $t_5$, 2 features moved from $C_4$ to $C_6$. Over next few time steps, $C_6$ became more homogeneous.
4.3.2 Web-Service Community Formation

We augmented dataset into evolutionary one, by modifying instances and features. We obtained distribution for each cluster and for \( t_1 \) and \( t_2 \), we modified 5% instances and features from each cluster using by randomly generating instances and features from distribution of clusters they belong to. For \( t_3 \) and \( t_4 \), we modified 5% instances and features from each cluster using by randomly generating instances and features from distribution of different cluster. At \( t_5 \), we added 5% new instances to cluster \( C_3 \) generated from distribution of \( C_3 \). Similarly, At \( t_6 \), we added 5% new features to \( C_1 \) generated from distribution of \( C_1 \). For \( t_7 \), we added 5% instances and features to instance and feature cluster \( C_2 \) from instance cluster \( C_4 \) and feature cluster \( C_5 \) respectively. At time-step \( t_8 \), we removed 1% instances and features each instance and feature cluster.

Figure 4.6: Comparison between accuracy of Evolutionary Higher order clustering (EHCC) and Higher order Clustering (HCC) for Web-service dataset

Similar to synthetic data, for web-service data algorithm shows ability to handle data dynamics. Figure 4.6 underlines algorithm’s ability to resists data changes. At time-step \( t_7 \), where we added instances as well as features to the data, static algorithm fail to perform, where as proposed algorithm has excellently handled data changes. Similarly for time-step \( t_8 \), when we removed instances and features from all clusters, our algorithm outperformed static version of the algorithm.
### 4.3.3 Text Co-clustering

We augmented dataset into evolutionary one in similar way as we did for the web-service dataset in section 4.3.2.

**Figure 4.7:** Comparison between accuracy of Evolutionary Higher order clustering (EHCC) and Higher order Clustering (HCC) for Text dataset, *England-Heart, re0*

**Figure 4.8:** Comparison between accuracy of Evolutionary Higher order clustering (EHCC) and Higher order Clustering (HCC) for Text dataset, *Graft-Phos, re0*
Through these experiments, we tried to test algorithm for text-datasets. Figures 4.7, 4.8, 4.9, and 4.10 further outline algorithm’s abilities to handle evolutionary data.

### 4.3.4 Image Co-clustering

For first experiment on image dataset, we increase the number of logs per category over the period of time $t_0$ to $t_{10}$. We mark all clusters distinctly with logs, so over period of time, we expect more tight intra-cluster association, and different clusters are more distinctly
identified. Then, we compare results for evolutionary algorithm with two different values of trade off factor $\alpha$, which equal to 0.8 and 0.2. This experiment also highlights algorithms ability of historic knowledge.

![Figure 4.11: Comparison between evolutionary higher order clustering algorithm (EHCC) and Static Higher order clustering algorithm (HCC), and comparison of performances of evolutionary algorithm with respect to trade-of factor $\alpha$](image)

In Figure 4.11, we compare evolutionary with static version of higher order co-clustering. As expected, evolutionary algorithm produces more accurate results than static version of higher-order co-clustering algorithm. In stead, over period of time, evolutionary algorithm produces more accurate results because of its capability of integration of historic knowledge. In later experiment, when we lowered value of trade-off factor, i.e. $\alpha = 0.3$, we gave more importance for historical data, so changes are further limited and algorithm restricted clustering towards historical one, hence lowering overall accuracy.
For second experiment, initially, we marked *African Lion* and *African Elephant* belong to same clusters. Over the period of time $t_0$ to $t_7$, we marked them separately into two clusters. We want to show, our proposed algorithm is able to handle cluster evolution over period of time. Again, we performed experiment for two different values of trade-off values to understand significance of integration of historic data.

![Figure 4.12: Change in number of clusters over period of time, for evolutionary higher order clustering algorithm (EHCC) and Static Higher order clustering algorithm (HCC); and comparison of performances of evolutionary algorithm with respect to trade-of factor $\alpha$.](image)

From Figure 4.12, we show that, algorithm resists change in data. Our algorithm indicates new cluster, i.e. $5^{th}$ cluster, is formed at time-step $t_2$, even though we have started marking $5^{th}$ from time-step $t_1$. So, new cluster is not formed till we have enough number of instances in new clusters for sufficient period of time. For trade-off value $\alpha = 0.3$, we
gave more importance for historical data, cluster change occurred more gradually. Hence, the fifth image cluster was detected one time-step later at $t_3$.

Figure 4.13: Number of instances in 5th cluster over period of time, for evolutionary higher order clustering algorithm (EHCC) and Static Higher order clustering algorithm (HCC); and comparison of performances of evolutionary algorithm with respect to trade-off factor $\alpha$.

In Figure 4.13, we show number of instances clustered into 5th. We can observe period time 5th cluster has become more prominent over period of time. As shown earlier, when we lower trade-off value, algorithm strongly opposes changes in structure of data.
5. Conclusion

I have proposed an evolutionary star-structured heterogeneous data co-clustering algorithm. The research addresses unexplored avenues in clustering evolving star-structured heterogeneous data. The algorithm augment the current data with the historical data using cost functions. Then it perform non-negative matrix factorization on the augmented current data to obtain clustering. To evaluate the proposed work, I have applied our approach to diverse domains: web-service community discovery, text mining and image clustering. Synthetic and real world and publicly available text and image datasets validate the proposed methodology.

Further experimentation will be necessary to determine possible applications based on my current research. An interesting direction would be tracking and analysis in social gaming applications, blogs or a mashup of RSS feeds with daily updates, users, and words to be clustered. Data dynamics has key effect on quality of the augmented matrix. So, additional efforts are required to improve ability to handle data dynamics. In the proposed approach, I have focused on a specific case of evolutionary heterogenous clustering. Further research is necessary to improve ability of the algorithm to handle general case of heterogenous data. The research will provide foundation for research on evolutionary heterogeneous data clustering, hence opening many avenues for evolutionary clustering applications. This research provides a road map for those that would venture to take on the endeavor of creating a novel algorithm in the evolving data mining field.
6. Acknowledgments

A grand thank you to Professor Rege, my committee, and Computer Science Department and Rochester Institute of Technology for their assistance with this thesis. I would like to take this opportunity to thank Hanghang Tong, Spiros Papadimitriou, Jimeng Sun, Philip Yu, and Christos Faloutsos for making Colibri [36] implementation available for our research.
Bibliography


[29] Manjeet Rege, Ming Dong, and Farshad Fotouhi. Co-clustering Documents and Words Using Bipartite Isoperimetric Graph Partitioning. Sixth International Conference on Data Mining ICDM06, pages 532–541, 2006.


[38] Lijun Wang, Manjeet Rege, Ming Dong, and Yongsheng Ding. Low-Rank Kernel Matrix Factorization for Large Scale Evolutionary Clustering. IEEE Transactions on Knowledge and Data Engineering, 99(PrePrints):1–15, 2010.


