

HIGHER ORDER MULTIPLE GRAPH FILTERING FOR STRUCTURED GRAPH LEARNING

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ABSTRACT

In the field of machine learning, multi-view clustering aims to reveal hidden clustering patterns across different data perspectives. However, traditional methods often struggle due to their reliance on low-order similarity data. To overcome this, we propose a new approach that integrates the learning of multiple graph filters, approximated through Chebyshev polynomials, with consensus structural graph learning into a unified framework. This method fully utilizes high-order statistical information from multiple data sources, thereby enhancing multi-view clustering. Comprehensive experiments conducted on multiple datasets consistently demonstrate significant performance improvements over traditional methods. Code is available at <https://github.com/lxd1204/HMGC>.

Index Terms— Multi-view clustering, high-order graph filtering, similarity graph, clustering performance

1. INTRODUCTION

In the field of machine learning, multiple graph clustering (MGC) is a key area that focuses on clustering data points represented by various graphs or networks. These graphs capture different aspects of the underlying data, aiming to reveal meaningful clusters that integrate information from all graphs [1, 2].

Nevertheless, traditional MGC methods have significant limitations, primarily their inability to consider high-order relationships among data points. This leads to a shortfall in capturing complex high-order dependencies within the data [3], especially in scenarios involving data with complex relationships that extend beyond pairwise comparisons.

Another common challenge in MGC is the lack of mechanisms to enhance the quality of input graphs during the clus-

tering process. In real-world scenarios, input graphs are often contaminated with noise or irrelevant data [4], and traditional methods[5] do not effectively resolve or improve the quality of these graphs, leading to suboptimal clustering performance due to noise or poorly constructed graphs.

To improve clustering performance, we propose a graph-based learning method that utilizes high-order Chebyshev polynomials to leverage complementary information between views [6] and local similarities within each view [7]. In our approach, we unify the learning of the consensus matrix and graph filters, integrating these processes into a single optimization framework. Within this framework, the consensus graph guides the learning of graph filters approximated by Chebyshev polynomials in each candidate graph. We also optimize candidate higher-order graph filters to effectively capture long-range relationships from the vertex domain and consider the influence of eigenvalues from the spectral domain [8]. This optimization results in a better consensus graph, allowing the learned consensus matrix to effectively guide the learning of graph filters. These innovations significantly enhance the accuracy and robustness of clustering results, especially when dealing with complex and noisy real-world data. Furthermore, this method has potential practical value in fields like molecular chemistry and social networks, where modeling complex relationships is crucial.

The main contributions of this paper are as follows:

- **Enhanced High-Order Graph Filtering:** Our method introduces high-order graph filters using Chebyshev polynomials, effectively capturing complex relationships among data points, a critical feature often lacking in traditional approaches.
- **Unified Optimization Framework:** We unify the learning of the consensus matrix and graph filters, establishing a bidirectional learning process that improves both components. This framework enhances the quality of the consensus graph and the accuracy of the graph

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filters.

- **Superior Multi-View Clustering Performance:** Through extensive experiments on multi-view data, our method consistently outperforms existing multi-view clustering approaches.

2. THE PROPOSED METHOD

2.1. First Order Neighbor Graph Construction

For a multi-view dataset consisting of v views, denoted as $\{\mathbf{X}^{(1)}, \dots, \mathbf{X}^{(v)}\}$, where $\mathbf{X}^{(v)} \in \mathbb{R}^{n \times d_v}$, with n representing the number of instances, and d_v indicating the feature dimension in the v -th view, it is crucial to construct high-quality graphs $\{\mathbf{S}^{(1)}, \dots, \mathbf{S}^{(v)}\}$, with $\mathbf{S}^{(v)} \in \mathbb{R}^{n \times n}$, for further clustering. In this paper, we adopt a simple yet effective neighbor assignment method [7]. The entries s_{ij} of the similarity graph matrix \mathbf{S}^v can be obtained as follows

$$s_{i,j}^v = \begin{cases} \frac{\mathbf{h}(\mathbf{x}_i^{(v)}, \mathbf{x}_{k+1}^{(v)}) - \mathbf{h}(\mathbf{x}_i^{(v)}, \mathbf{x}_j^{(v)})}{\sum_{j'=1}^k (\mathbf{h}(\mathbf{x}_i^{(v)}, \mathbf{x}_{k+1}^{(v)}) - \mathbf{h}(\mathbf{x}_i^{(v)}, \mathbf{x}_{j'}^{(v)}))}, & j \leq k, \\ 0, & j > k. \end{cases} \quad (1)$$

where $\mathbf{h}(\cdot, \cdot)$ measures the Euclidean distance between two samples and k is the neighborhood size.

2.2. Higher Order Chebyshev Polynomials

Given an affinity matrix \mathbf{S} , which represents pairwise similarities or weights between nodes in a graph, Chebyshev polynomials $\{T_i(\mathbf{S})\}$ are defined as a sequence of polynomials, where i varies from 0 onwards. These polynomials are computed recursively as follows:

$$\begin{aligned} T_0(\mathbf{S}) &= \mathbf{I}, \quad T_1(\mathbf{S}) = \mathbf{S}, \\ T_t(\mathbf{S}) &= 2\mathbf{S}T_{t-1}(\mathbf{S}) - T_{t-2}(\mathbf{S}), \quad \text{for } t \geq 2. \end{aligned}$$

\mathbf{I} signifies the identity matrix, and \mathbf{S} represents the affinity matrix. These Chebyshev polynomials are element-wise operations on \mathbf{S} , finding applications in various graph signal processing tasks.

In contrast to the first-order affinity graph \mathbf{S} , Chebyshev polynomials offer distinct advantages in graph signal processing. They provide a higher-order representation of graph data, allowing for the capture of intricate relationships beyond pairwise connections. Chebyshev filtering proves computationally efficient, especially for large graphs, while maintaining numerical stability to reduce potential errors. Moreover, Chebyshev filters enable localized filtering, facilitating the examination of specific local patterns within the graph, and they efficiently extract spectral information, making them versatile tools for diverse graph-based applications. These advantages establish Chebyshev polynomials as a potent choice for graph signal processing tasks.

In practical applications, Chebyshev polynomials can be employed to filter a graph signal \mathbf{x} using the following expression:

$$\mathbf{y} = \sum_{t=0}^{\hat{t}} \beta_t T_t(\mathbf{S}) \mathbf{x} \quad (2)$$

Here, \mathbf{y} represents the filtered signal, β_t denotes filter coefficients, and \hat{t} signifies the order of the Chebyshev filter.

2.3. Multiple Higher Order Structural graph learning

For each affinity graph, we can build a set of Chebyshev polynomials in the form of

$$\left\{ \sum_{t=0}^{\hat{t}} \beta_t^1 T_t(\mathbf{S}^{(1)}), \sum_{t=0}^{\hat{t}} \beta_t^2 T_t(\mathbf{S}^{(2)}), \dots, \sum_{t=0}^{\hat{t}} \beta_t^{(v)} T_t(\mathbf{S}^{(v)}) \right\}. \quad (3)$$

We aim to minimize the weighted sum of squared differences between the linear combinations of Chebyshev polynomials applied to the affinity matrices $\mathbf{S}^{(v)}$ and the final consensus affinity matrix \mathbf{A} by solving the following optimization problem for the v -th view:

$$\begin{aligned} \min_{\beta^v, \mathbf{A}} \quad & \left\| \sum_{t=0}^{\hat{t}} \beta_t^v T_t(\mathbf{S}^{(v)}) - \mathbf{A} \right\|_2^2 \\ \text{s.t.} \quad & 0 \leq a_{ij} \leq 1, \sum_{j=1}^n a_{ij} = 1. \end{aligned} \quad (4)$$

Here, β_t^v is the coefficient associated with each Chebyshev polynomial, and a_{ij} is the weight associated with the elements of matrix \mathbf{A} , with $0 \leq a_{ij} \leq 1$ for all i and j .

Subsequently, we aggregate the weighted errors across all views and orders of Chebyshev polynomials by solving the following optimization problem:

$$\begin{aligned} \min_{\alpha, \beta, \mathbf{A}} \quad & \sum_{v=1}^m \alpha_v^2 \left\| \sum_{t=0}^{\hat{t}} \beta_t^v T_t(\mathbf{S}^{(v)}) - \mathbf{A} \right\|_2^2 \\ \text{s.t.} \quad & 0 \leq \alpha_v \leq 1, \sum_{v=1}^m \alpha_v = 1, 0 \leq a_{ij} \leq 1, \sum_{j=1}^n a_{ij} = 1, \end{aligned} \quad (5)$$

where α_v represents the weight assigned to the v -th view.

To enforce the target matrix \mathbf{A} to have the desired number of connected components, we introduce the constraint on the rank of the Laplacian matrix $\mathbf{L}_\mathbf{A}$ as $\text{rank}(\mathbf{L}_\mathbf{A}) = n - c$ based on Ky Fan's theorem. Furthermore, we introduce the sum of the top c smallest eigenvalues of $\mathbf{L}_\mathbf{A}$ to control its rank.

The higher order multiple graph filtering for structured graph learning and clustering (HMGC) method can be sum-

marized as follows:

$$\begin{aligned}
\min_{\alpha, \beta, \mathbf{A}, \mathbf{F}} \quad & \sum_{v=1}^m \alpha_v^2 \left\| \sum_{t=0}^{\hat{t}} \beta_t^v T_t(\mathbf{S}^{(v)}) - \mathbf{A} \right\|_2^2 + \lambda \text{tr}(\mathbf{F}^T \mathbf{L}_A \mathbf{F}) \\
\text{s.t.} \quad & 0 \leq \alpha_v \leq 1, \sum_{v=1}^m \alpha_v = 1, \\
& 0 \leq a_{ij} \leq 1, \sum_{j=1}^n a_{ij} = 1, \mathbf{F}^T \mathbf{F} = \mathbf{I}_c.
\end{aligned} \quad (6)$$

$\mathbf{F} \in \mathbb{R}^{n \times c}$ consists of c eigenvectors corresponding to c eigenvalues of \mathbf{L}_A . In HMGC, we use Chebyshev polynomials to minimize the weighted sum of squared differences between linear combinations of these polynomials applied to multiple affinity matrices $\mathbf{S}^{(v)}$ and a consensus matrix \mathbf{A} . We achieve this through two optimization steps, optimizing Chebyshev coefficients and \mathbf{A} for each view and then aggregating errors across all views and polynomial orders. HMGC provides a powerful framework for structured graph learning and clustering, allowing control over the number of connected components in the final consensus matrix \mathbf{A} . In summary, HMGC enhances graph-based data analysis by combining higher-order Chebyshev polynomials and multi-view affinity matrices.

3. OPTIMIZATION PROCESS

In this paper we adopt the block coordinate descend method to update a single variable while keeping other variables fixed.

Update α . Fixing β , \mathbf{F} , and \mathbf{A} , the rest problem w.r.t. α reduces to:

$$\min_{\alpha} \sum_{v=1}^m \alpha_v^2 e_v \quad \text{s.t.} \quad 0 \leq \alpha_v \leq 1, \sum_{v=1}^m \alpha_v = 1, \quad (7)$$

where $e_v = \left\| \sum_{t=0}^{\hat{t}} \beta_t^v T_t(\mathbf{S}^{(v)}) - \mathbf{A} \right\|_2^2$. We can obtain its closed-form solution as follows:

$$\alpha_v = \frac{e_v^{-1}}{\sum_{v'=1}^m e_{v'}^{-1}}. \quad (8)$$

Update β . Fixing α , \mathbf{F} , and \mathbf{A} , the rest problem w.r.t. $\beta \in \mathbb{R}^{\hat{t} \times m}$ is column decoupled. The sub-problem of the v -th column w.r.t. β^v can be written as:

$$\min_{\beta^v} \beta^{vT} \mathbf{H}^{(v)} \beta^v + \beta^{vT} \mathbf{f}^v, \quad (9)$$

where $\mathbf{H}^{(v)} \in \mathbb{R}^{\hat{t} \times \hat{t}}$ with $\mathbf{H}_{ij}^{(v)} = \text{tr}(T_i(\mathbf{S}^{(v)})^T T_j(\mathbf{S}^{(v)}))$, and $\mathbf{f}^v \in \mathbb{R}^{\hat{t} \times 1}$ with $f_t^v = -2\text{tr}(T_t(\mathbf{S}^{(v)})^T \mathbf{A})$. Eq.(9) can be easily solved by off-the-shelf solvers.

Update \mathbf{A} . Fixing α , β , and \mathbf{F} , the rest problem w.r.t. \mathbf{A} reduces to:

$$\min_{\mathbf{A}} \left\| \mathbf{A} - \mathbf{B} \right\|_2^2 \quad \text{s.t.} \quad 0 \leq a_{ij} \leq 1, \sum_{j=1}^n a_{ij} = 1, \quad (10)$$

Table 1. Summary of the Data Sets

ID	Data Name	Samples	Features	Classes
D1	3SOURCES	169	3560,3631,3068	6
D2	TEXAS	187	1703,187	5
D3	CORNELL	195	1703,195	5
D4	COIL	1440	1024,944,4096,576	20
D5	100LEAVES	1600	64,64,64	100
D6	NUSWIDE	2000	64,225,144,73,128	31
D7	MNIST4	4000	30,9,30	4
D8	PBMC	4271	100,200,400,100,200,400,64,128,256	8
D9	SCENE	4485	20,59,40	15
D10	SUNRGBD	10335	4096,4096	45

where $\mathbf{B} = \frac{\sum_{v=1}^m \alpha_v^2 \sum_{t=0}^{\hat{t}} \beta_t^v T_t(\mathbf{S}^{(v)}) - \frac{\lambda}{4} \mathbf{D}_F}{\sum_{v=1}^m \alpha_v^2}$ and $\mathbf{D}_F \in \mathbb{R}^{n \times n}$ denotes the pairwise distance on \mathbf{F} . Eq.(10) is row decoupled and each sub-problem can be solved by the Euclidean projection on the simplex [7].

Update \mathbf{F} . Fixing α , β , and \mathbf{A} , the rest problem w.r.t. \mathbf{F} reduces to:

$$\min_{\mathbf{F}} \text{tr}(\mathbf{F}^T \mathbf{L}_A \mathbf{F}) \quad \text{s.t.} \quad \mathbf{F}^T \mathbf{F} = \mathbf{I}_c. \quad (11)$$

The optimal solution for \mathbf{F} corresponds to the c smallest eigenvalues of \mathbf{L}_A and their corresponding eigenvectors.

After the convergence of the iterative algorithm, the final clustering results can be obtained from \mathbf{A} . We omit the convergence and complexity analysis due to space limitation.

4. EXPERIMENTS

4.1. Benchmark Datasets

We conducted experiments on 10 benchmark datasets, primarily covering two categories: documents and images. In the document category, we included the news dataset 3SOURCES¹ and TEXAS², which encompasses web pages and hyperlinks. For the image category, it includes 100LEAVES³ (Comprising 100 types of plant images), NUSWIDE [9] (Network images), MNIST [10] (Handwritten images), COIL⁴ (Color images), PBMC⁵ (Cell images), SCENE⁶, and CORNELL⁷ (Object images), as well as SUNRGBD [11] (RGB images related to scene understanding). The detailed information of these datasets is shown in Table 1.

4.2. Experiment Setup

In our experiments, we evaluate the performance of various clustering algorithms on a diverse set of benchmark datasets.

¹<http://mlg.ucd.ie/datasets/3sources.html>

²<https://starling.utdallas.edu/datasets/webkb>

³<https://archive.ics.uci.edu/ml/datasets/One-hundred+plant+species+leaves+data+set>

⁴<https://www.cs.columbia.edu/CAVE/software/softlib/coil-20.php>

⁵<https://satijalab.org/seurat/vignettes.html>

⁶<https://figshare.com/articles/dataset/15-SceneImageDataset/7007177>

⁷http://www.cs.cornell.edu/textasciitildecristian/Cornell_Movie-Dialogs_Corpus.html

Table 2. Accuracy results on all datasets. Bold indicates the best results, and underline indicates the second-best results.

Methods	D1	D2	D3	D4	D5	D6	D7	D8	D9	D10
AWP	62.72	50.27	42.05	69.86	78.88	15.15	60.65	63.59	36.63	17.23
MCGC	74.56	55.61	52.82	80.69	72.75	14.90	80.25	55.07	14.74	18.23
GMC	69.23	52.94	52.82	80.35	82.38	14.90	92.03	62.61	14.00	12.77
LMVSC	54.44	55.61	50.77	65.83	60.63	13.70	64.18	57.01	35.88	18.49
OPLF	60.80	55.61	50.77	54.37	75.19	14.05	87.37	54.88	37.53	8.92
LSRMSC	63.31	54.55	48.72	59.72	3.81	14.00	50.58	46.66	22.92	-
2CMV	34.32	54.10	49.66	67.50	70.86	12.45	72.51	53.45	33.36	18.65
EOMSC	33.14	56.68	44.62	60.97	42.06	16.02	88.65	67.82	32.95	23.70
AONGR	52.07	58.82	47.69	69.10	88.19	15.50	64.93	56.52	40.69	19.98
HMGC	76.92	63.64	56.05	95.12	93.16	16.13	92.35	68.51	41.53	<u>20.29</u>

These datasets, summarized in Table 1, encompass a wide range of characteristics, including the number of samples, features, and classes.

To demonstrate the effectiveness of our proposed method, we conducted comparative experiments with nine state-of-the-art multi-view clustering approaches. These approaches include AWP [12], MCGC [13], GMC [14], LMVSC [15], 2CMV [16], OPLF [5], AONGR [17], EOMSC [18] and LSRMSC [19]. Across all datasets, we set the number of clusters equal to the number of classes. For our method, we simply fix the neighborhood size regularization $k = 10$ and conduct grid search on the parameter $\lambda \in [10^{-3}, \dots, 10^3]$ and the order of ChebyshevPolynomials $\hat{t} \in [3, \dots, 10]$. The clustering performance is assessed through the utilization of two commonly employed metrics: Accuracy (ACC) and Normalized Mutual Information (NMI). Due to space limitations, we only report the clustering accuracy in Table 2 and omit the results for other metrics time consumption and parameter sensitively analysis.

4.3. Experimental Results Analysis

The impractical time complexity of LSRMSC on the D10 restricts its feasible execution within a reasonable timeframe. In contrast, our proposed HMGC exhibits superior performance across all datasets. This is evident from consistently higher accuracy scores, as shown in Table 2. Notably, on challenging datasets (e.g., D4 and D5), HMGC achieves significantly better accuracy compared to its counterparts. Furthermore, as shown in Fig. 1, we present the t-SNE [20] results of AWP, OPLF, LMVSC, and our HMGC on D8. We can see that our method achieves better embedding results because it can more clearly partition the data into different categories. This underscores the robustness and effectiveness of HMGC in achieving accurate and reliable clustering results.

4.4. Ablation Study

We introduce a first-order graph clustering method denoted as MGC, which utilizes only $\{T_1(\mathbf{S}^{(1)}), T_1(\mathbf{S}^{(2)}), \dots, T_1(\mathbf{S}^{(m)})\}$ as defined in Eq. (6). The results of first-order MGC and

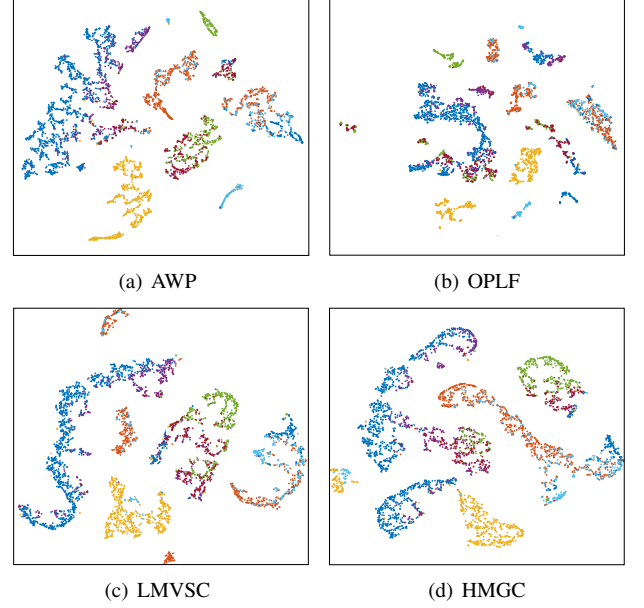


Fig. 1. We respectively present the t-SNE results of embeddings using AWP, OPLF, LMVSC, and our HMGC on D8.

higher-order HMGC are presented in Table 3. These results clearly demonstrate that leveraging higher-order graphs with optimized coefficient learning significantly enhances clustering performance.

Table 3. Ablation Study on First and Higher order MGC

Dataset	ACC		NMI	
	MGC	HMGC	MGC	HMGC
D1	72.78	76.42	63.48	73.48
D2	61.50	63.64	31.14	35.70
D3	53.33	56.05	36.83	41.00
D4	87.36	95.12	93.90	97.48
D5	87.59	93.16	94.04	96.88
D6	14.38	16.13	14.87	15.94
D7	92.23	92.35	81.02	81.42
D8	64.84	68.51	56.56	60.44
D9	39.98	41.53	39.12	42.07
D10	17.54	20.29	18.78	23.78

5. CONCLUSION

HMGC has introduced a promising approach in multi-graph clustering, demonstrating exceptional capability in uncovering hidden structures within complex datasets. Utilizing Chebyshev polynomials built from adjacency matrices, our method effectively captures the high-order, nonlinear relationships in the data. This innovation not only boosts clustering performance but also enhances the model’s flexibility and robustness when dealing with complex data structures. In the future, we plan to explore the spectral properties of Chebyshev polynomials in multi-graph clustering tasks and extend their application to other specific uses.

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