Adaptive Weighted Spectral Clustering

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Outline

1. Cluster Ensemble Selection
2. The proposed method
3. Experimental Results
4. Summary
Clustering

- Finding groups of objects such that the objects in a group will be similar (or related) to one another and different from (or unrelated to) the objects in other groups.

Intra-cluster distances are minimized

Inter-cluster distances are maximized
Challenge

Weighted Spectral Cluster Ensemble
Brain Extraction Problem

There are two approaches.
Brain Extraction Problem

Weighted Spectral Cluster Ensemble
Brain Extraction Problem

Our consideration >>

In practice >>

Weighted Spectral Cluster Ensemble
We need a robust diversity metric.

The performance of CES is significantly sensitive to the threshold value.

How can we find the threshold value in a real-world application?
Outline

1. Cluster Ensemble Selection
2. The proposed method
3. Experimental Results
4. Summary
The proposed framework

Weighted Spectral Cluster Ensemble
Main Idea of mapping function is transforming data to stable dimensions.
Step 1: The Mapping Function

Algorithm 1 The Mapping Function

Input: Data set $\hat{X} \in \mathbb{R}^{m \times n} = \{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n\}$,
- $d$ as number of features:
  - $d = 0$ is considered for deactivating the feature selection
Output: Mapped data set $Y$
Method:

1. Calculating simple average $\hat{X}$ by using (1).
2. Calculating $X$ by using (2).
3. Calculating $R = \mathbb{E}\{XX^T\} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T$.
4. Calculating $\Lambda$ and $Q$ as eigenvalues/vectors of $R$.
5. Sorting $Q$ based on descending values of $\lambda$.
6. if $d$ is not zero ($d \neq 0$)
   then selecting $[1, d]$ features of $Q$, and sorting as $Q_d$,
   else $Q_d = Q$, $d = m$.
   end if
7. Return $Y = Q_d^T \hat{X}$.

<< calculating the zero-mean of data
Step 1: The Mapping Function

Algorithm 1 The Mapping Function

**Input:** Data set $\hat{X} \in \mathbb{R}^{m \times n} = \{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n\}$,
    
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**Output:** Mapped data set $Y$

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5. Sorting $Q$ based on descending values of $\lambda$.
6. if $d$ is not zero ($d \neq 0$)
    
    then selecting $[1, d]$ features of $Q$, and sorting as $Q_d$,
    
    else $Q_d = Q$, $d = m$.

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Weighted Spectral Cluster Ensemble
Step 1: The Mapping Function

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end if

7. Return $Y = Q_d^T \hat{X}$.
Step 1: The Mapping Function

Algorithm 1 The Mapping Function

**Input:** Data set \( \hat{X} \in \mathbb{R}^{m \times n} = \{ \hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n \} \),

- \( d \) as number of features:
- \( d = 0 \) is considered for deactivating the feature selection

**Output:** Mapped data set \( Y \)

**Method:**

1. Calculating simple average \( \bar{X} \) by using (1).
2. Calculating \( X \) by using (2).
3. Calculating \( R = \mathbb{E}\{XX^T\} = \frac{1}{n} \sum_{i=1}^{n} x_i x_i^T \).
4. Calculating \( \Lambda \) and \( Q \) as eigenvalues/vectors of \( R \).
5. Sorting \( Q \) based on descending values of \( \lambda \).
6. **if** \( d \) is not zero (\( d \neq 0 \))
   - **then** selecting \([1, d]\) features of \( Q \), and sorting as \( Q_d \),
   - **else** \( Q_d = Q, \ d = m \). << the optional feature selection
7. Return \( Y = Q_d^T X \).
Step 1: The Mapping Function

**Algorithm 1 The Mapping Function**

**Input:** Data set $\hat{X} \in \mathbb{R}^{m \times n} = \{\hat{x}_1, \hat{x}_2, \ldots, \hat{x}_n\}$, $d$ as number of features: $d = 0$ is considered for deactivating the feature selection

**Output:** Mapped data set $Y$

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   else $Q_d = Q$, $d = m$.
end if

7. Return $Y = Q_d^T \hat{X}$.

<< apply mapping function on data points

Weighted Spectral Cluster Ensemble
Step 2: Generating individual results

- Transforming data point to similarity matrix $S$

$$S_{i,j} = \begin{cases} 
exp \left( -\frac{\|y_i - y_j\|_2}{\phi^2} \right) & \text{if } i \neq j \\
0 & \text{if } i = j
\end{cases}$$

$\phi$ is the scaling parameter for controlling how rapidly affinity $S_{i,j}$

$\phi$ can be calculated automatically by Ng et al., 2001.
Step 2: Generating individual results

Algorithm Two Kernels Spectral Clustering (TKSC)

**Input:** Distance matrix $A$, Number of clusters $K$

**Output:** Partitional result $P$, Modular result $M$

**Method:**

1. Generate similarity matrix $S$ by using $A$
2. Generate diagonal matrix $D$ by using $S$.
3. Generate $L_P$ by applying $S$ and $D$ on $L_P = I - D^{1/2}SD^{1/2}$
4. Generate $L_M$ by using $S$ and $D$ on $L_M = D - S$
5. Generate the matrix $V$ as eigenvectors of $L_p$.
6. Generate $U$ as normalized $V$ by using $SQ_i = \left( \sum_{i=1}^{M} V_{i1} \times V_{i2} \right)^{1/2} + \epsilon$ and $U_{ij} = V_{ij} \times SQ_i$

7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\max(L_M)}L_M$
8. $P = kmeans(U, K)$

<< calculating the similarity and its diagonal matrix
### Algorithm: Two Kernels Spectral Clustering (TKSC)

**Input:** Distance matrix $A$, Number of clusters $K$  
**Output:** Partitional result $P$, Modular result $M$  
**Method:**

1. Generate similarity matrix $S$ by using $A$
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7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\text{max}(L_M)} L_M$
8. $P = kmeans(U, K)$

$<<$ calculating the second Laplacian matrix as the modular kernel

Weighted Spectral Cluster Ensemble
Step 2: Generating individual results

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7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\max(L_M)} L_M$
8. $P = kmeans(U, K)$

<< calculating the eigenvectors of $L_P$
Step 2: Generating individual results

Algorithm  Two Kernels Spectral Clustering (TKSC)

**Input:** Distance matrix $A$, Number of clusters $K$

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7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\max(L_M)}L_M$
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Normalizing the eigenvectors >>
Step 2: Generating individual results

Algorithm Two Kernels Spectral Clustering (TKSC)

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7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\max(L_M)}L_M$ << Normalizing the modular result

8. $P = kmeans(U, K)$

Weighted Spectral Cluster Ensemble
Step 2: Generating individual results

**Algorithm**  Two Kernels Spectral Clustering (TKSC)

**Input:** Distance matrix $A$, Number of clusters $K$

**Output:** Partitional result $P$, Modular result $M$

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7. Generate $M$ by applying $L_M$ on $M = \frac{1}{\max(L_M)}L_M$
8. $P = kmeans(U, K)$

<<< calculating the partitional results

Weighted Spectral Cluster Ensemble
Step 3: Diversity evaluation

- This paper proposes Normalized Modularity for calculating the diversity by exploiting the partitional and modular results.
- This metric employs the concept of Expected Value for calculating the diversity.
- This metric is a new branch of famous Modularity, which is an effective metric in the field of community detection, for general clustering problem.

\[ NM(P^l, M) = \frac{1}{2} + \frac{1}{4z} \sum_{ij} \left[ \Gamma_{ij} - \frac{\sigma_i \sigma_j}{2z} \right] \Theta (c_i, c_j) \]

\[ \Gamma_{ij} = \begin{cases} 0 & \text{if } M_{ij} = 0 \\ 1 & \text{Otherwise} \end{cases} \quad \Theta (c_i, c_j) = \begin{cases} 1 & \text{if } c_i = c_j \\ 0 & \text{Otherwise} \end{cases} \]

- \( P \) is Partitional result. \( M \) is Modular result.
- \( z \) is sum of all cells in the matrix \( M \) (\( m = \sum M_{ij} \)).
- \( c_i \) and \( c_j \) are the number of classes for the i-th and j-th instances in the \( P \).
- \( \sigma_i, \sigma_j \) show the degree of i-th and j-th nodes in the graph of the \( M \).
- This diversity evaluation is \( 0 \leq NM \leq 1 \).
Step 4: Evidence Accumulation Clustering

- $\alpha$ represents the number of clusters shared by objects with indices $i$ and $j$.

- $\beta$ is the number of partitions in which this pair of instances ($i$ and $j$) is simultaneously presented.

- In fact, EAC considers that the weights of all algorithms results are the same.

Weighted Spectral Cluster Ensemble
Step 4: Weighted EAC

- **WEAC:**
  \[
  c(i,j) = \frac{\sum_{\alpha(i,j)} \rho_{i,j}}{\beta(i,j)}
  \]

- Although the weight can have different definitions in the other applications, this paper uses average of **Normalized Modularity** of two algorithms as follows for combining individual results:

- **Final co-association matrix:**
  \[
  \rho_{ij} = \frac{1}{2}(NM_i + NM_j)
  \]

\[
\xi = WEAC(\zeta) = \begin{pmatrix}
  c(1,1) & c(1,2) & \ldots & c(1,n) \\
  c(2,1) & c(2,2) & \ldots & c(2,n) \\
  \vdots & \vdots & \ddots & \vdots \\
  c(i,1) & c(i,2) & c(i,j) & c(i,n) \\
  \vdots & \vdots & \vdots & \vdots \\
  c(n,1) & c(n,2) & \ldots & c(n,n)
\end{pmatrix}
\]
Outline

1. Cluster Ensemble Selection
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3. Experimental Results
4. Summary
Experiment Setup

- **Data Set**: we employ 26 standard data
  - Image based data set
    - Alzheimer's Disease data set (MRI and PET images from human brain)
    - USPS: a handwriting data set
  - Document based data set
    - 20 Newsgroups, Reuters-21578
    - More than 20 data set mostly from UCI data repository

- **Algorithms**:
  - Individual Clustering methods:
    - Spectral clustering (Ng et al., 2001), MLE (Chen el al., 2014)
  - Cluster Ensemble (Selection) methods:
    - APMM (Alizadeh et al., 2014), WOCCE (Alizadeh et al., 2015), SMI (Romano et al., 2014), BGCM (Gao et al., 2013)
## Performance Analysis

Weighted Spectral Cluster Ensemble

<table>
<thead>
<tr>
<th>Data Sets</th>
<th>Spectral</th>
<th>MLE</th>
<th>APMM</th>
<th>WOCCE</th>
<th>SMI</th>
<th>BGCM</th>
<th>WSCE</th>
</tr>
</thead>
<tbody>
<tr>
<td>20 Newsgroups</td>
<td>14.31±2.14</td>
<td>21.89±1.02</td>
<td>28.03±0.87</td>
<td>32.62±0.52</td>
<td>29.14±0.91</td>
<td>40.61±0.83</td>
<td>52.06±0.17</td>
</tr>
<tr>
<td>ADNI-MRI-C1</td>
<td>39.24±0.21</td>
<td>39.84±0.42</td>
<td>48.01±0.56</td>
<td>48.82±0.37</td>
<td><strong>50.69±0.69</strong></td>
<td>45.54±0.99</td>
<td>49.53±0.19</td>
</tr>
<tr>
<td>ADNI-MRI-C2</td>
<td>32.72±0.98</td>
<td>26.32±0.67</td>
<td>39.93±0.29</td>
<td>40.22±0.44</td>
<td>38.32±0.41</td>
<td><strong>42.62±1.04</strong></td>
<td>41.14±0.71</td>
</tr>
<tr>
<td>ADNI-PET-C1</td>
<td>43.71±0.52</td>
<td>37.96±0.87</td>
<td>48.37±0.82</td>
<td>49.19±0.26</td>
<td>49.45±0.62</td>
<td>42.1±0.78</td>
<td><strong>52.05±0.37</strong></td>
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<td>ADNI-PET-C2</td>
<td>37.27±0.23</td>
<td>37.91±0.83</td>
<td>38.53±0.17</td>
<td>39.43±0.79</td>
<td>41.76±0.47</td>
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<td><strong>43.11±0.42</strong></td>
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<td>ADNI-FUL-C1</td>
<td>42.63±0.63</td>
<td>42.62±0.58</td>
<td>47.22±0.93</td>
<td>48.82±0.41</td>
<td>47.93±0.83</td>
<td>48.56±1.26</td>
<td>49.06±0.36</td>
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<td>ADNI-FUL-C2</td>
<td>39.51±1.19</td>
<td>41.06±0.17</td>
<td>50.09±0.35</td>
<td>49.39±0.63</td>
<td>49.16±0.26</td>
<td>46.91±0.42</td>
<td><strong>50.11±0.09</strong></td>
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<td>Arcene</td>
<td>58.31±1.22</td>
<td>64.19±0.498</td>
<td>66.28±0.216</td>
<td>65.16±0.32</td>
<td>67.14±0.93</td>
<td>64.23±0.28</td>
<td><strong>73.34±0.92</strong></td>
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<td>Bala. Scale</td>
<td>49.21±0.87</td>
<td>52.76±0.12</td>
<td>52.65±0.67</td>
<td>54.88±0.61</td>
<td>59.98±0.812</td>
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<td>Breast Can.</td>
<td>94.88±1.14</td>
<td>82.65±0.342</td>
<td>96.04±0.88</td>
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<td>99.12±0.62</td>
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<td>Bupa</td>
<td>56.72±1.18</td>
<td>53.98±0.274</td>
<td>55.07±0.28</td>
<td>57.02±0.46</td>
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<td>53.17±0.21</td>
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<tr>
<td>CNAE-9</td>
<td>65.32±0.43</td>
<td>77.72±0.591</td>
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<td>79.2±0.579</td>
<td>74.25±0.614</td>
<td>80.12±0.459</td>
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<td>Galaxy</td>
<td>31.24±0.67</td>
<td>34.25±0.872</td>
<td>33.72±0.36</td>
<td>35.88±0.81</td>
<td>35.21±0.413</td>
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<td>Glass</td>
<td>45.78±0.87</td>
<td>50.32±0.42</td>
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<td>Half Ring</td>
<td>80.61±1.15</td>
<td>73.91±0.762</td>
<td>80±0.42</td>
<td>87.2±0.14</td>
<td>71.19±0.621</td>
<td>98.37±0.59</td>
<td><strong>99.92±0.08</strong></td>
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<td>Ionosphere</td>
<td>69.71±0.67</td>
<td>25.67±0.53</td>
<td>70.94±0.13</td>
<td>70.52±0.132</td>
<td>70.87±0.226</td>
<td>73.67±0.341</td>
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<td>Iris</td>
<td>83.45±0.82</td>
<td>89.02±0.61</td>
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<td>Optdigit</td>
<td>54.19±0.45</td>
<td>73.81±0.69</td>
<td>77.1±0.841</td>
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<td>Pendigits</td>
<td>53.94±0.25</td>
<td>59.36±0.31</td>
<td>47.4±0.699</td>
<td>58.68±0.18</td>
<td>63.74±0.37</td>
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<td>Reuters-21578</td>
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<td>52.58±1.92</td>
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<td>SA Hart</td>
<td>69.59±0.08</td>
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<td>70.91±0.42</td>
<td>68.7±0.46</td>
<td>70.05±0.51</td>
<td><strong>73.92±0.72</strong></td>
<td>72.8±0.82</td>
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<td>Sonar</td>
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<td>57.64±0.47</td>
<td>52.06±0.873</td>
<td><strong>61.29±0.11</strong></td>
</tr>
<tr>
<td>Statlog</td>
<td>42.87±0.62</td>
<td>52.35±0.79</td>
<td>54.88±0.528</td>
<td>55.77±0.719</td>
<td>53.73±0.52</td>
<td>55.76±0.591</td>
<td><strong>57.92±0.26</strong></td>
</tr>
<tr>
<td>USPS</td>
<td>62.67±0.13</td>
<td>59.72±0.62</td>
<td>63.91±0.94</td>
<td>65.21±0.69</td>
<td>68.73±0.66</td>
<td>65.38±1.02</td>
<td><strong>70.37±0.01</strong></td>
</tr>
<tr>
<td>Wine</td>
<td>73.09±1.38</td>
<td>83.81±0.41</td>
<td>64.6±0.231</td>
<td>71.34±0.542</td>
<td>88.46±0.71</td>
<td>87.34±0.24</td>
<td><strong>90.44±0.02</strong></td>
</tr>
<tr>
<td>Yeast</td>
<td>32.96±0.71</td>
<td>30.49±0.63</td>
<td>31.06±0.245</td>
<td>32.76±0.268</td>
<td>35.19±0.57</td>
<td>28.12±0.462</td>
<td><strong>36.92±0.81</strong></td>
</tr>
</tbody>
</table>
The effect noisy data on the performance of the proposed method

- **Arcene**
  - WSCE
  - BGCM
  - SMI
  - APMM
  - WOCCE

- **CNAE-9**

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**Noise Analysis**

**Weighted Spectral Cluster Ensemble**
Missed-values Analysis

- The effect missed-values on the performance of the proposed method

![Missed-values Analysis](image)

**Weighted Spectral Cluster Ensemble**
Outline

1. Cluster Ensemble Selection
2. The proposed method
3. Experimental Results
4. Summary
There are two challenges in Cluster Ensemble Selection:
- Proposing a robust consensus metric(s) for diversity evaluation.
- Estimating optimum parameters in the thresholding procedure for selecting the evaluated results.

This paper introduces a novel solution for solving mentioned challenges:
- Mapping function and Optional feature selection (preparing raw data)
- Two Kernel Spectral Clustering (TKSC) algorithm (generating individual results)
- Normalized Modularity (estimating diversity)
- Weighted Evidence Accumulation Clustering (generating final result)

An extensive experimental study is performed by comparing with individual clustering methods as well as cluster ensemble (selection) methods on a large number of data sets.

Results clearly show the superiority of our approach on both normal data sets and those with noise or missing values.

In the future, we will develop a new version of Normalized Modularity for estimating the diversity of Partitional results, directly.
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