Relevance Analysis based on graph theory and spectral analysis


Abstract—Category 1. We present a new method for relevance analysis based on spectral information, which is done from a graph theory point of view. This method is carried out by using Gaussian Kernels instead of conventional quadratic forms and then avoiding the need of a linear combination-based representation. For this end, it is implemented an extended approach for relevance analysis using alternative Kernels, in this case, exponential ones. For assessing the proposed method performance, it is applied a clustering algorithm commonly used and recommended by literature: normalized cuts based clustering. Experimental results are obtained from the processing of well known image and toy data bases. Results are comparable with those reported in the literature.

Index Terms— Eigen-solution, exponential kernels, Gaussian kernels, graph theory, spectral clustering.

I. INTRODUCTION

In pattern recognition context, determining the most relevant features is, in almost all cases, a crucial stage to design an automatic classification system. On this regard, many approaches have been proposed that are focused on several problems, such as compactness guarantee, separability, classification performance, dimensionality reduction, feature extraction, among others [1]. For instance, the conventional principal component analysis (PCA) is applied to determine how many features are relevant according to an explained variance criterion [2], [3]. One of the greatest disadvantages of the variance analysis-based methods is that they cannot successfully be applied on problems where features are highly uncorrelated, which for difficult classification data do not guarantee separability, as well as large data.

By other hand, there exist many methods for solving the previous mentioned problems but they are usually computationally expensive [4]. In general, there is no a generic established method for relevance analysis that can be applied to different types of data, achieving a good tradeoff between computational cost and performance in terms of classification. It has been proposed many methods that accomplish an admissible performance but increasing the computational cost. In contrast, there exist other methods that require low computational cost but decreasing classification performance.

In this work, a new method for relevance analysis, applied on difficult data bases employing spectral information about data, is presented that is done from a graph theory point of view. This method is carried out by using Gaussian Kernels instead of conventional quadratic forms and then avoiding the need of a linear combination quadratic forms. For this end, it is implemented an extended approach for relevance analysis using alternative Kernels, in this case, exponential ones. For assessing the proposed method performance, it is applied a clustering algorithm commonly used and recommended by literature: normalized cuts based clustering. Experimental results are obtained from the processing of well known image and toy data bases. Results are comparable with those reported in the literature.

II. THEORETICAL BACKGROUND

A. Multi-class Spectral Clustering (MCSC)

A weighted graph can be represented as \(G = (V, E, \Omega)\), where \(V\) is the set of either nodes, \(E\) is the edge set, and \(\Omega\) represents the relationship among nodes, that is the kernel matrix or affinity matrix as well. Given that, each affinity matrix entry \(\omega_{ij} \in \Omega \in \mathbb{R}^{N \times N}\) represents the weight of the edge between \(i\)-th and \(j\)-th element, it must be a non-negative value. Value \(N\) is the number of considered samples or nodes. In addition, for a non-directed graph, it holds that \(\omega_{ij} = \omega_{ji}\). Therefore, affinity matrix must be chosen as symmetric and positive semi-definite one. In spectral analysis, term \(V = \{1, \ldots, n\}\) represents the indices of data set to be grouped. The aim of spectral clustering is to decompose \(V\) into \(K\) disjoint subsets, then, \(V = \bigcup_{k=1}^{K} V_k\) and \(V_l \cap V_k = \emptyset, \forall l \neq k\), such decomposition is done, commonly, by using spectral information and orthonormal transformations. Data to be clustered are to be denoted as \(X \in \mathbb{R}^{N \times d} = [x_1^\top, \ldots, x_N^\top]^\top\), where \(x_i \in \mathbb{R}^d\) is the \(i\)-th sample related to \(i\)-th node.

In matrix representation terms, the aim of MCSC is to determine a binary indicator matrix \(M = (m^{(1)}\top, \ldots, m^{(K)}\top)\), where each vector \(m^{(k)}\) is a column vector formed by data point membership regarding cluster \(k\). Each entry \(ik\) of matrix \(M\) is defined as

\[
m_{ik} = [i \in V_k], \quad i \in V, \quad k = 1, \ldots, K,
\]

where notation \([\cdot]\) stands for a binary indicator - it equals to 1 if its argument is true and, otherwise, 0. Also, because each node can only belong into one partition, the condition

\[
m_{ij} + m_{ji} = 1, \quad \forall i, j \in V
\]
$M \mathbf{1}_K = \mathbf{1}_N$ must be satisfied, where $\mathbf{1}_d$ is a $d$-dimensional all ones vector.

Then, the well-known $k$-way normalized cuts-based clustering, described in [5], can be written as:

$$\max_M \varepsilon_M = \frac{1}{K} \frac{\text{tr}(\mathbf{M}^T \Omega \mathbf{M})}{\text{tr}(\mathbf{M}^T \mathbf{D} \mathbf{M})}$$  \hspace{1cm} (1a)

subject to $M \in \{-1, 1\}^{N \times K}$, $M \mathbf{1}_K = \mathbf{1}_N$  \hspace{1cm} (1b)

where $\mathbf{D} \in \mathbb{R}^{N \times N}$ is the degree matrix related to weights or affinity matrix, defined as $\mathbf{D} = \text{Diag}(\Omega \mathbf{1}_N)$. Notation $\text{Diag}(\cdot)$ denotes a diagonal matrix formed by its argument vector. Expressions (1a) and (1b) are the formulation of normalized cuts optimization problem, named (NCPM).

### III. RELEVANCE ANALYSIS-BASED DATA PROJECTION

Let us consider the notation given in Table III.

<table>
<thead>
<tr>
<th>Term</th>
<th>Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original data matrix</td>
<td>$X$</td>
<td>$X \in \mathbb{R}^{n \times n}$</td>
</tr>
<tr>
<td>Rotation matrix</td>
<td>$Q$</td>
<td>$Q \in \mathbb{R}^{p \times d}, Q^T Q = I_d$</td>
</tr>
<tr>
<td>Truncated rotation matrix</td>
<td>$Q$</td>
<td>$Q \in \mathbb{R}^{p \times p}, Q^T Q = I_p, p &lt; d$</td>
</tr>
<tr>
<td>Projected data</td>
<td>$Y$</td>
<td>$Y \in \mathbb{R}^{n \times p}, Y = XQ$</td>
</tr>
<tr>
<td>Truncated projected data</td>
<td>$Y'$</td>
<td>$Y' \in \mathbb{R}^{n \times p}, Y = XQ$</td>
</tr>
<tr>
<td>Reconstructed data</td>
<td>$X$</td>
<td>$X \in \mathbb{R}^{n \times d}, X = YQ'$</td>
</tr>
</tbody>
</table>

For obtaining a rotation matrix $\hat{Q}$ such that $\hat{Y}$ contains the projected vectors that most contribute to the explained variance, in [6] is introduced the following optimization problem:

$$\min_{\hat{Q}} \|X - \hat{X}\|_A^2 = \max_{\hat{Q}} \text{tr}(\hat{Q}^T X^T AX \hat{Q})$$ \hspace{1cm} (2)

subject to $\hat{Q}^T \hat{Q} = I_d$ \hspace{1cm} (3)

where $A$ is a semidefinite positive matrix.

The eigenvectors associated to the $p$ largest eigenvalues of $X^T AX$, i.e., $Q = \text{eig}(X^T AX)$ is a feasible solution. The $p$ value is established by means of an accumulated variance criterion. As can be inferred from equation 2, when matrix $A$ is chosen as $I$ we have the standard PCA. When $A$ is chosen as a weighted covariance, WPCA versions are accomplished. Because affinity matrix contains the relationship values of all data points, we propose to select matrix $A$ as the affinity $\Omega$ that can be understood as an estimation of a covariance matrix.

### IV. EXPERIMENTAL SETUP

Database of public domain numerical matrix format is used for the analysis and study of the proposed method. Table I summarizes the real data used for the analysis showing the variability of selected databases.

Experiments are carried out on two well-known database collections: Firstly, a toy data comprising the following several data sets (4Gaussians, Bulls eye 2 circulos, Bulls eye 3 circulos, dataset1, dataset2, dataset3, dataset 4grupos, dataset 5grupos, HappyFace) as is shown in the Figure 1.

![Figure 1. Considered artificial databases](image)

Secondly, a real databases comprising the following several data sets(iris, 80x, auto_mpg, malaysia, biomed, breast, cbands, chomo, diabetes, ecoli, glass, heart, ionsphere, liver satellite, sonar, soybean1, soybean2, spirals, twonorm, ringnorm, wine, mfeat_fad, mfeat_fou, mfeat_kar, mfeat_pix, mfeat_zer, mfeat_mor).

Estimation of the group number, $k$, is based on calculation of the eigenvector set of the affinity matrix [9]. In particular, the scaled exponential affinity matrix $\Omega = \omega_{ij}$ is employed that holds elements defined as follows: [10]

$$\omega_{ij} = \begin{cases} 
\exp\left( -\frac{d^2(x_i, x_j)}{\sigma_i \sigma_j} \right), & i \neq j \\
0, & i = j 
\end{cases}$$ \hspace{1cm} (4)

where $X \in \mathbb{R}^{n \times p} = (x_1^T, \ldots, x_n^T)^T$ is the data matrix, $x_i \in \mathbb{R}^p$ is its corresponding $i$-th data point, $\sigma_i = d(x_i, x_N)$, $x_N$ denotes the $N$-th nearest neighbor, and $d(\cdot, \cdot)$ stands for Euclidian distance. The value of $N$ is experimentally set to be 2.

Table II shows the clustering performance measures with their description.

Lastly, testing within experimental framework is carried out by employing MATLAB Version 7.10.0(R2010a) in a standard PC Acer Npilfy TM 802 AMD processor V120, 2.2 GHz and 2 GB RAM memory.
V. RESULTS AND DISCUSSION

Table III shows the numerical results obtained for each of the components of toy data sets, in general we can note that the exponential kernels works significantly better than the conventional method for relevance analysis. This fact can be appreciated in the following components: 4Gaussians, Bulls_eye_3_circulos, dataset2, dataset3, dataset_4grupos and dataset_5grupos.

Table IV shows the numerical results obtained for each of the components of real databases, in general we can note that the exponential kernels works significantly better than the conventional method for relevance analysis. This fact can be appreciated in the following components: iris, 80x, biomed and breast.

Then, be shown the images of relevance analysis of somethings toy and real databases.

- **Toy databases**
- **4 Gaussians**: for this case we can note that the second is the most relevant feature.
- **Bulls eye 2 circulos**: we can note that the second is the most relevant feature.
- **Happy Face**: we can note that the second is the most relevant feature.

Figure 2 show the boxplot for the toy databases; we can note that the three boxplots are symmetric, symmetrical to the right and symmetrical to the right respectively, interquartile range is 1.43, 6.92 and 15.94 respectively. The top quartile has its maximum point in 1.45, 6.92 and 24.6; we can note that the exponential kernels works significantly better than the conventional method for relevance analysis.

- **Real databases**:
  - **iris**: we can note that the first is the most relevant feature.
  - **80x**: As show the image the most relevant features are the second and sixth.
  - **auto_mpg**: In this case there is a difference between the third feature is the most relevant and all other.
  - **malaysia**: In this case there is a difference between the second feature is the most relevant and all other.
  - **biomed**: we can note that the fifth is the most relevant feature.
  - **breast**: we can note that the first is the most relevant feature.

Figure 3 shows the boxplot for the Real databases; we can note that the three boxplots are symmetrical to the right, interquartile range is 44.36, 25.6 and 26.5 respectively. The top quartile has its maximum point in 45.3, 26 and 26.5.
A. Clustering Index

• Toy databases

It can be noted in Figure 4 that the proposed method to artificial data bases, is satisfactory, because in the Table V shows the corresponding values, which have a value near to one, this indicates the effectiveness of the exponential Kernels, that shows a good measure of clustering. Also we can say that linear projection improves the clustering performance.

As it can be seen in the Figure 5, the distribution obtained from the toy database can be distributed as follows:

– Input: Presents a non-symmetrical distribution because the median is very close to the upper face, so it is easy to see that approaches the third quartile for this reason the data have a distribution skewed to the left. One can appreciate the outliers of the distribution, these values may represent the effects of extraneous causes that is, measurement error or error in any of the records, these are significant with a red cross in the coordinates (1, 1). Interquartile range is 0.002, which shows a dispersal in the minimum database, which carries a degree of detachment rate compared to its average value. On the other hand, we see that the top quartile has a peak 1, which indicates that the method is useful, obtaining a satisfactory method.

– Output: As input, does not present a symmetrical distribution, the median is observed that in this case is the quartile 3 of the picture, it is concluded that in this case presents an asymmetry to the left. Presents a minimum value of 0.998, and in this case not observed outliers which may cause error in the output of the grouping. Interquartile range is 0.002, this result shows the dispersal in the databases as input, indicating that the degree of detachment is a little higher with respect to its mean value. The proposed method is generally satisfactory, because it is close to unity.

• Real databases

By the other hand according to the previws information in Figure 6, gives the results of the Real database. Table VI shows the respective values of both original and obtained by the exponential kernel. We conclude that for this database the method presents a behavior and a high effectiveness, because these measures are near to unity, as the results of the toy databases is possible to say that improves the linear projection clustering performance too.

<table>
<thead>
<tr>
<th>Original</th>
<th>Spectral Clustering</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000</td>
<td>0.9998</td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
</tr>
<tr>
<td>1.0000</td>
<td>0.9999</td>
</tr>
<tr>
<td>0.9999</td>
<td>1.0000</td>
</tr>
<tr>
<td>1.0000</td>
<td>0.9998</td>
</tr>
<tr>
<td>1.0000</td>
<td>1.0000</td>
</tr>
</tbody>
</table>
TABLE VI
PLOT FOR CLUSTERING COHERENCE OF REAL DATA

<table>
<thead>
<tr>
<th>Original</th>
<th>Spectral Clustering</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0000</td>
<td>0.9592</td>
</tr>
<tr>
<td>0.9020</td>
<td>0.8081</td>
</tr>
<tr>
<td>1.0000</td>
<td>0.8961</td>
</tr>
<tr>
<td>0.9984</td>
<td>0.6025</td>
</tr>
<tr>
<td>0.9788</td>
<td>0.8373</td>
</tr>
<tr>
<td>0.9906</td>
<td>0.9634</td>
</tr>
</tbody>
</table>

As it can be seen in the Figure 7, the distribution obtained from the real database can be distributed as follows:

**Input:** Did not show a symmetrical distribution, also mediated is very close to the upper face, so it is easy to see that approaches the third quartile for this reason the data have a distribution skewed to the left. It can be noted the outliers of the distribution, these values may represent the effects of extraneous causes that is, measurement error or error in any of the registers, these are significant with a red cross in the coordinates (1, 0.923). Intercuartil range is 0.009, which shows dispersal in the minimum database, which carries a degree of distance rate compared to its average value.

**Output:** As input, does not present a symmetrical distribution, the median is observed that in this case is near to the underside box, therefore it is concluded that in this case presents an asymmetry to the right. Presents a minimum value of 0.6, and in this case not observed outliers which may cause error in the output of the grouping. Intercuartil range is 0.151, this result shows the dispersal in the databases is a little higher than the input, indicating that the degree of detachment is a little higher with respect to its mean value. The upper level is at 0.963. The proposed method is generally satisfactory, because it is near to unity.

VI. CONCLUSIONS AND FUTURE WORK

We introduced a variant of a linear projection approach for relevance analysis by means of a generalize distance regarding affinity matrix. Projection improves the clustering performance and can be extended as a feature selection method obtaining a relevance vector.

As a future work, more spectral analysis methods and affinity measures will be explored to design an adequate relevance analysis approach keeping a good trade-off between the number of resultant features and performance.

VII. ACKNOWLEDGEMENT

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REFERENCES


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