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CLASSIFICATION OF MULTIGRAPHS VIA SPECTRAL TECHNIQUES[1]

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Abstract

Classification problems of the vertices of large multigraphs (hypergraphs or weighted graphs) can be easily handled by means of linear algebraic tools. For this purpose notion of the Laplacian of multigraphs will be introduced, the eigenvectors belonging to k consecutive eigenvalues of which define optimal k-dimensional Euclidean representation of the vertices. In this way perturbation results are obtained for the minimal $(k+1)$-cuts of multigraphs (where k is an arbitrary integer between 1 and the number of vertices). The $(k+1)$-variance of the optimal k-dimensional representatives is estimated from above by the k smallest positive eigenvalues and by the gap in the spectrum between the k^{th} and $(k+1)^{\mathrm{th}}$ positive eigenvalues in increasing order. These results are of statistical character. However, they are useful and well-adopted to automatic computation in the case of large multigraphs when one is not interested in strict structural properties and, on the other hand, usual enumeration algorithms are very time-demanding.

Keywords: Laplacian spectra of graphs, Euclidean representations, optimal k-partitions, perturbation results.

1. Introduction

Hypergraphs and weighted graphs (in the sequel referred to as multigraphs) often arise when multiple or pairwise connections between objects of a finite set are of interest. For the investigation of some structural properties (e.g. k-colourability, minimal–maximal cuts) there exist well-known enumeration algorithms and theoretical results as well, e.g. HOFFMAN (1970), CVETKOVIĆ, DOOB, SACHS (1979), SIMONOVITS (1984), ALON (1986). But in the case of large multigraphs – when one is not interested in the strict fulfilment of the investigated property – perturbation results can be proved by means of linear algebraic tools.

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For this purpose optimal Euclidean representation of multigraphs are introduced together with their Laplacian (Section 3). The Laplacian is a positive semidefinite Hermitian matrix which has a physical meaning in special cases. First it was defined by FIEDLER (1973) for ordinary graphs.

Our purpose is merely by the investigation of the Laplacian spectra and of the usual metric distances of the representatives in a multidimensional Euclidean space to characterize the following structural property of a given multigraph: there exists an integer k (between 1 and the number of vertices) for which there is a k-partition of the set of vertices in such a way that most of the hyperedges (or in the case of weighted graphs edges with large weights) belong to the same cluster of the k-partition (Sections 4 and 5). Relationships between spectral gaps of the Laplacian and variances of the clusters can also be proved (Section 6). Some properties of Laplacian spectra and examples can be found in Section 7.

The above property often arises in the multivariate statistical analysis when mutually dependent binary variables are classified in such a way that objects having many binary properties in common would possibly belong to the same cluster. The iterative algorithm – introduced in Chapter 8 – applies the spectral technique in one step of the iteration, while in the other steps the partitions and the dimensions are determined. The algorithm is part of the DISTAN (DIscrete STatistical ANalysis) program package, see RUDAS (1992). Weighted graphs are used e.g. for the description of neural networks, see MC ELIECE et al. (1987), KOMLÓS and PATURI (1989).

3-dimensional representation of hypergraphs has a special meaning in chemistry when we are looking for spacial arrangement of compounds by merely knowing the connections between their atoms. The quadratic form to be introduced in Section 3 has a physical interpretation in the investigation of the atomic structure, where the energy of the elementary particles is minimized. The spectrum of the Laplacian also gives information on the atomic orbitals (Section 9).

2. Notations

A hypergraph H is defined by the pair (V, E), where V is a finite set and $E \subset 2^V$ consists of its selected subsets. V is called the set of the vertices and E is the set of the edges of the hypergraph H. A vertex is denoted by $v \in V$ and an edge (for brevity a hyperedge will be called simply an edge) by $e \in E$. Let $|V| = n$ and $|E| = m$. Then H can be given by its $n \times m$ *vertex-edge incidence matrix* $\mathbb{A}$ with entries $a_{ji} = \mathcal{I}(v_j \in e_i)$, where

$$\mathcal{I}(v \in e) = \begin{cases} 1, & \text{if} \quad v \in e \\ 0, & \text{otherwise} \end{cases}$$

and the relation $v \in e$ denotes that the vertex v is incident with the edge e. Furthermore let us denote by $|e|$ the number of vertices contained by the edge $|e|$.

A weighted graph G is defined by the pair $(V, \mathbb{W})$, where $V := \{v_1, \ldots v_n\}$ is the set of its vertices and $\mathbb{W}$ is the *weight matrix* of the edges of G. The diagonal entries of the $n \times n$ matrix $\mathbb{W}$ are zero, while the nondiagonal entry w_{ij} is the weight assigned to the edge $\{v_i, v_j\}$ and $w_{ij} = w_{ji} \geq 0$, $i \neq j$. (If the vertices v_i and v_j are not adjacent, the weight w_{ij} is zero.)

An ordinary graph is a special case of a weighted graph the weight matrix being its adjacency matrix (its $\{i, j\}^{\text{th}}$ entry is 1, if the vertices v_i and v_j are connected and 0, otherwise).

3. Spectra and Euclidean Representation of Multigraphs

Let the hypergraph H on vertex-set $\{v_1, \ldots, v_n\}$ and edge-set $\{e_1, \ldots, e_m\}$ be given by its $n \times m$ incidence matrix A. Let k $(1 \leq k \leq n)$ be a fixed integer. We are looking for k-dimensional representatives $\mathbf{x}_j$, $(j = 1, \ldots, n)$ and $\mathbf{y}_i$, $(i = 1, \ldots, m)$ of the vertices and edges, respectively, so that

$$\sum_{j=1}^{n} \mathbf{x}_j \mathbf{x}_j^T = \mathbb{I}_k \tag{3.1}$$

and the sum of the costs of edges

$$Q = \sum_{i=1}^{m} K(e_i) = \sum_{i=1}^{m} \sum_{j=1}^{n} a_{ij} \|\mathbf{x}_j - \mathbf{y}_i\|^2 \tag{3.2}$$

in this representation is minimized, where the cost $K(e_i)$ of the edge e_i is defined by

$$K(e_i) := \sum_{j=1}^{n} a_{ji} \|\mathbf{x}_j - \mathbf{y}_i\|^2, \tag{3.3}$$

the k-dimensional variance of the representatives of its vertices from the representative of the edge in question. For an individual edge its cost is minimized if we substitute the centre of gravity of the representatives of its vertices for its representative. After performing this substitution for every edge, the decreased objective function Q will be the quadratic form

$$L(\mathbf{X}) = \sum_{i=1}^{n} \sum_{j=1}^{n} \left[\frac{1}{2} \sum_{e \in E} \mathcal{I}(v_i \in e) \mathcal{I}(v_j \in e) \frac{1}{|e|} \right] \|\mathbf{x}_i - \mathbf{x}_j\|^2 = \sum_{i=1}^{n} \sum_{j=1}^{n} c_{ij} \mathbf{x}_i^T \mathbf{x}_j \tag{3.4}$$

with

$$c_{ij} = \begin{cases} -\sum\limits_{e\in E} \mathcal{I}(v_i \in e)\mathcal{I}(v_j \in e)\frac{1}{|e|}, & \text{if} \quad i \neq j, \\ s_i - \sum\limits_{e\in E} \mathcal{I}(v_i \in e)\frac{1}{|e|} = s_i' - \sum\limits_{\substack{e\in E \\ |e|>1}} \mathcal{I}(v_i \in e)\frac{1}{|e|}, & \text{if} \quad i = j, \end{cases} \tag{3.5}$$

where $s_i' = \#\{e \in E \ : \ v_i \in e, \ |e| > 1\}$. The matrix of the quadratic form (3.4) is called the **Laplacian** of the hypergraph H, and it is denoted by $\mathbf{C}$. It can also be written as

$$\mathbf{C} = \mathbf{D}_v - \mathbf{A}\mathbf{D}_e^{-1}\mathbf{A}^T,$$

where $\mathbf{D}_v$ and $\mathbf{D}_e$ are the valency matrices of the vertices and edges, respectively.

The quadratic form $L(\mathbf{X})$ is equal to $\operatorname{tr} \mathbf{X}\mathbf{C}\mathbf{X}^T$, and it is to be minimized on $\mathbf{X}\mathbf{X}^T = \mathbf{I}_k$. As the $n \times n$ matrix $\mathbf{C}$ is symmetric and positive semidefinite, by means of a theorem for the extrema of quadratic forms – RAO (1979) – the following **Representation Theorem** can be proved, see BOLLA (1989):

THEOREM 3.1 *The minimum of the cost function* (3.2) *conditioned on* (3.1) is

$$\sum_{j=1}^{k} \lambda_j, \tag{3.6}$$

where $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of the Laplacian $\mathbf{C}$ and it is attained, when the k-dimensional Euclidean representation $\mathbf{X}$ of the vertices contains pairwise orthonormal eigenvectors corresponding to the k smallest eigenvalues of $\mathbf{C}$ in its rows. If such an $\mathbf{X}$ is denoted by $\mathbf{X}^*$, the optimal choice for the k-dimensional Euclidean representation $\mathbf{Y}$ of the edges is $\mathbf{Y}^* = \mathbf{X}^*\mathbf{A}\mathbf{D}_e^{-1}$. □

Let $\mathbf{R}$ be a $k \times k$ orthogonal matrix ($\mathbf{R}\mathbf{R}^T = \mathbf{I}_k$). Then neither the objective function nor the constraint is effected by the substitution $\mathbf{X}' = \mathbf{R}\mathbf{X}$. Thus, together with an optimal $\mathbf{X}^*$, the matrix $\mathbf{R}\mathbf{X}^*$ is optimal too. But apart from k-dimensional rotations, in the case of distinct eigenvalues the optimal $\mathbf{X}^*$ is uniquely determined by the Laplacian $\mathbf{C}$. Otherwise their rows can be chosen appropriately within the eigenspaces belonging to the multiple eigenvalues.

In the future, whenever k-dimensional representatives $\mathbf{x}^*$-s and $\mathbf{y}^*$-s constituting the columns of any optimal $\mathbf{X}^*$, $\mathbf{Y}^*$ pair are assigned to the vertices and to the edges, respectively, we speak of *optimal k-dimensional* **Euclidean representation** of the hypergraph H.

Since for optimal representations of the vertices and those of the edges the relation $\mathbf{Y}^* = \mathbf{X}^*\mathbf{A}\mathbf{D}_e^{-1}$ holds, an optimal representation $\mathbf{X}^*$ of the vertices uniquely determines an optimal representation of the hypergraph H, and by the formula (3.4) it gives a minimal variance arrangement of the vertices in the k-dimensional Euclidean space.

We remark that the dimension k does not play an important role here yet, since for any k $(1 \leq k < n)$ an optimal $(k+1)$-dimensional Euclidean representation is obtained from an optimal k-dimensional one by introducing a subsequent eigenvector in the rows of $\mathbf{X}$. Or vice versa, a k-dimensional optimal Euclidean representation is the projection of the $(k+1)$-dimensional one onto the subspace spanned by eigenvectors corresponding to the k smallest eigenvalues.

It can be seen from the formulas of (3.5) that the loops (edges with $|e| = 1$) do not contribute to the entries of the Laplacian matrix, so in the future only hypergraphs without loops will be considered.

Let us also notice that the Laplacian is always singular since all row sums are 0. The eigenvector corresponding to a single zero eigenvalue is $\frac{1}{\sqrt{n}}\mathbf{e}$, where $\mathbf{e}$ is the n-dimensional vector of 1-s. In this case a k-dimensional Euclidean representation is realized in the $(k-1)$-dimensional subspace of R^k orthogonal to the vector $\mathbf{e}$. It is well known that the multiplicity of the zero as an eigenvalue of a hypergraph without loops and isolated vertices is equal to the number of its connected components. In this case the spectrum consists of the spectra of its components, so only spectra of connected hypergraphs are of interest. But in the case of connected hypergraphs one can ask how many edges must be removed so that the hypergraph be not connected or consist of k components. How the strongly connected sub-hypergraphs can be recognized on the basis of optimal Euclidean representations? These problems are discussed in the subsequent sections.

In the case of weighted graphs let d_j denote the sum of the weights of the edges incident with the vertex v_j. Suppose that $d_j > 0$, $(j = 1, \ldots, n)$ and $\mathbf{D} = \operatorname{diag}(d_1, \ldots, d_n)$ be the diagonal matrix with d_j-s in its main diagonal.

Let $k (1 \leq k < n)$ be a fixed integer and let the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in R^k$ satisfy the constraints $\sum_{j=1}^n \mathbf{x}_j \mathbf{x}_j^T = \mathbf{I}_k$ and $\sum_{j=1}^n \mathbf{x}_j = 0$. Here the vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n$ are regarded as k-dimensional representatives of the vertices. Let $\mathbf{X} := (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ be the $k \times n$ matrix containing the vectors $\mathbf{x}_j$-s as its columns. Let us define the quadratic form

$$Q := \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} \|\mathbf{x}_i - \mathbf{x}_j\|^2 = \operatorname{tr} \mathbf{X}\mathbf{C}\mathbf{X}^T, \tag{3.7}$$

where the $n \times n$ matrix $\mathbf{C}$ is equal to $\mathbf{D} - \mathbf{W}$. This $\mathbf{C}$ is also symmetric, singular and positive semidefinite. We call it the *Laplacian* of the weighted graph G.

We remark that a weighted graph can be always assigned to a hypergraph in such a way that their Laplacians be the same as follows:

$$w_{ij} = w_{ji} = \sum_{e \in E} \mathcal{I}(v_i \in e)\mathcal{I}(v_j \in e)\frac{1}{|e|}, \qquad (1 \leq i < j \leq n).$$

Let us denote by

$$0 = \lambda_0 \leq \lambda_1 \leq \cdots \leq \lambda_{n-1}$$

the eigenvalues of the Laplacian $\mathbf{C}$. A **Representation Theorem** similar to that for hypergraphs can be proved: the minimum of Q constrained on $\mathbf{X}\mathbf{X}^T = \mathbf{I}_k$ and $\sum_{j=1}^{n} \mathbf{x}_j = 0$ is $\sum_{j=1}^{k} \lambda_j$ and it is attained for $\mathbf{X}^* = (\mathbf{u}_1, \ldots, \mathbf{u}_k)^T$, where $\mathbf{u}_1, \ldots, \mathbf{u}_k \in R^n$ are k pairwise orthonormal eigenvectors corresponding to the eigenvalues $\lambda_1, \ldots, \lambda_k$ of the matrix $\mathbf{C}$. The column vectors $\mathbf{x}_1^*, \ldots, \mathbf{x}_n^*$ of any optimal $\mathbf{X}^*$ are called *optimal k-dimensional representatives* of the vertices and then we speak of *optimal k-dimensional Euclidean representation* of the weighted graph G.

The above representation can be extended to weighted graphs, the vertices of which are weighted too, as follows. Let G be a weighted graph with weight matrix $\mathbf{W}$ of the edges, the vertex v_j of which has the weight s_j, $(j = 1, \ldots, n)$ and $\mathbf{S} := \operatorname{diag}(s_1, \ldots, s_n)$. Now the quadratic form Q of (3.7) is minimized subject to the constraints that $\sum_{j=1}^{n} s_j \mathbf{x}_j \mathbf{x}_j^T = \mathbf{X}\mathbf{S}\mathbf{X}^T = \mathbf{I}_k$ and $\sum_{j=1}^{n} s_j \mathbf{x}_j = 0$. Since Q can be written as

$$\operatorname{tr} \mathbf{X}\mathbf{C}\mathbf{X}^T = \operatorname{tr}(\mathbf{X}\mathbf{S}^{1/2})[\mathbf{S}^{-1/2}\mathbf{C}\mathbf{S}^{-1/2}](\mathbf{X}\mathbf{S}^{1/2})^T, \tag{3.8}$$

the minimum of Q on the above constraint is $\sum_{j=1}^{k} \kappa_j$ — where $0 = \kappa_0 \leq \kappa_1 \leq \cdots \leq \kappa_{n-1}$ are the eigenvalues of the symmetric, singular, positive semidefinite matrix in brackets — and it is attained for the representation $\mathbf{X}^* = (\mathbf{u}_1, \ldots, \mathbf{u}_k)^T \mathbf{S}^{-1/2}$ of the vertices, where $\mathbf{u}_1, \ldots, \mathbf{u}_k$ are k pairwise orthonormal eigenvectors corresponding to the k smallest positive eigenvalues of the so-called *weighted Laplacian* $\mathbf{C}_S := \mathbf{S}^{-1/2}\mathbf{C}\mathbf{S}^{-1/2}$. With other words the $k \times n$ matrix $(\sqrt{s_1}\mathbf{x}_1^*, \ldots, \sqrt{s_n}\mathbf{x}_n^*)$ — where the column vectors $\mathbf{x}_1^*, \ldots, \mathbf{x}_n^*$ of any optimal $\mathbf{X}^*$ are called optimal k-dimensional representatives of the vertices — contains the above eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_k$ in its rows.

We remark that in the case of the weighted graph G on vertex set V the weight matrix $\mathbf{W}$ can be regarded as a symmetric measure on the product of measure spaces $(I, \mathcal{A})$, $(I, \mathcal{A})$, where $I = \{1, 2, \ldots, n\}$ and $\mathcal{A}$

is the generated σ-algebra. The probabilities of elementary events are $d_1, d_2, \dots, d_n$. Let $\mathbb{W}(I) = 1$ and the symmetricity of $\mathbb{W}$ means that $\mathbb{W}(A \times B) = \mathbb{W}(B \times A)$ for any $A, B \in \mathcal{A}$ pairs. Hence $\mathbb{D} = \{d_1, d_2, \dots, d_n\}$ is just the marginal of the joint distribution $\mathbb{W}$. Let us denote by $\mathbb{P} : L_2(I, \mathcal{A}, \mathbb{D}) \to L_2(I, \mathcal{A}, \mathbb{D})$ the operator taking the conditional expectation according to the joint distribution $\mathbb{W}$. Its matrix form is $\mathbb{D}^{-1/2}\mathbb{W}\mathbb{D}^{-1/2}$, therefore the above $\mathbb{C}_D$ is just $\mathbb{I}_n - \mathbb{P}$ and ϱ-s are like *canonical correlations.*

4. Structural Properties of Hypergraphs by Means of Spectral Techniques

Let $H = (V, E)$, $|V| = n$, $|E| = m$ be a hypergraph without loops and multiple edges, its eigenvalues being $0 = \lambda_1 \leq \lambda_2 \cdots \leq \lambda_n$ in increasing order. Now we shall give upper and lower bounds for combinatorial measures characterizing k-partitions of the vertex set of H by means of the k smallest eigenvalues, where k is any natural number between 2 and n. First of all let us introduce the following notions:

DEFINITION 4.1 A k-tuple $(V_1, \dots, V_k)$ of non-empty subsets of V is called a *k-partition* of the set of vertices, if $V_i \cap V_j = \emptyset$ for $i \neq j$ and $\cup_{i=1}^{k} V_i = V$. Sometimes a k-partition is denoted by P_k, while the set of all k-partitions by $\mathcal{P}_k$. The **volume** $v(P_k)$ of the k-partition $P_k = (V_1, \dots, V_k)$ is defined by

$$v(P_k) := \sum_{e \in E} \frac{1}{|e|} \sum_{1 \leq i < j \leq k} a_i(e)\, a_j(e)$$

and its **weighted volume** $u(P_k)$ by

$$u(P_k) := \sum_{e \in E} \frac{1}{|e|} \sum_{1 \leq i < j \leq k} \left(\frac{1}{n_i} + \frac{1}{n_j} \right) a_i(e)\, a_j(e),$$

where $a_i(e) = |e \cap V_i|$ and $n_i = |V_i|$.

The **minimal k-cut** of H is defined by

$$\mu_k(H) = \min_{P_k \in \mathcal{P}_k} v(P_k), \tag{4.1}$$

while the **minimal weighted k-cut** by

$$\nu_k(H) = \min_{P_k \in \mathcal{P}_k} u(P_k). \tag{4.2}$$

DEFINITION 4.2 The *cut set* of the k-partition $P_k = (V_1, \dots, V_k)$ consists of those edges e for which $|e \cap V_i| \neq \emptyset$ holds for at least two different parts of P_k, and it is denoted by $H(P_k)$. The k-partition P_k defines a *colouring* c of the vertices in the following way: $c(v) := i$, if $v \in V_i$. An edge e is said to be *multi-coloured* in this colouring, if it contains two different vertices v, v' such that $c(v) \neq c(v')$. Thus, the cut set $H(P_k)$ consists of the multi-coloured edges. $H(P_k^*)$ is called a *minimal k-sector* of H, if

$$|H(P_k^*)| = \min_{P_k \in \mathcal{P}_k} |H(P_k)|,$$

and its cardinality is denoted by $\theta_k(H)$. THEOREM 4.3 *For the sum of the k smallest eigenvalues of the hypergraph H the upper and lower estimations*

$$c_n \theta_k(H) \leq \sum_{j=1}^{k} \lambda_j \leq \nu_k(H) \tag{4.3}$$

hold, where $c_n = \frac{6}{n(n^2-1)}$. For the proof see BOLLA (1989). The upper bound shows that the existence of k relatively small eigenvalues is a necessary condition for the existence of a good classification (with a small minimal weighted cut). Thus, the spectrum can give us some idea about the choice of the number k of the clusters for which good colouring may exist. But the spectrum itself does not say anything about the optimal k-partition, moreover, it does not give a sufficient condition for the existence of a good clustering. The lower bound in (4.3) depends on the constant c_n, and there are graphs for which the lower bound is attained in order of magnitude. E.g. for lattices and spiders (see Section 7, Examples 7.8 and 7.9), which cannot be classified into k clusters in a sensible way.

For a graph G it is the same estimate as given by FIEDLER (1973). He has also given an upper bound for λ_2 by the edge-connectivity $e(G)$ of the graph G. As $\nu_2(H) \leq \frac{n}{n-1}\mu_2(H)$ and $\mu_2(H) = \frac{1}{2}e(G)$, for the second smallest eigenvalue of graphs the upper bound $\nu_2(G)$ is asymptotically sharper than $\frac{1}{2}e(G)$, the estimate of Fiedler.

Now we want to recognize optimal k-partitions by means of classification of k-dimensional representatives of the vertices in an optimal k-dimensional Euclidean representation of the hypergraph. The classification is performed by the k-means method introduced by MAC QUEEN (1967). We shall be confined to the case, when a 'very' well-separated k-partition of the above k-dimensional points exists.

DEFINITION 4.4 *A k-partition $P_k = (V_1, \ldots, V_k)$ is called a well-separated k-partition of the vertex set V in the k-dimensional Euclidean representation $\mathbb{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ of the vertices, if for the colouring c belonging to P_k the relation $\alpha(P_k) > 1$ holds, where*

$$\alpha(P_k) := \frac{\min\limits_{c(v_i) \neq c(v_j)} \|\mathbf{x}_i - \mathbf{x}_j\|}{\max\limits_{c(v_i) = c(v_j)} \|\mathbf{x}_i - \mathbf{x}_j\|}. \tag{4.4}$$

(In the case when there exists a well-separated k-partition of the k-dimensional points $\mathbf{x}_1, \dots, \mathbf{x}_n$, DUNN (1974) has proved its uniqueness, and he has given an algorithm to determine the k well-separated clusters of $\mathbf{x}_j$-s. Dunn has also proved that the larger $\alpha(P_k)$ is, the better the separation and the quicker the algorithm is.)

THEOREM 4.5 *Assume that for some $k < n$ there exists a well-separated k-partition of the vertex set V, for the clusters of which the diameters are at most ε, where $\varepsilon < \frac{1}{2\sqrt{n}}$ is a small positive number. Then*

$$\nu_k(H) \le q^2 \sum_{j=1}^{k} \lambda_j, \tag{4.5}$$

where $q = 1 + \frac{2\varepsilon}{1-\varepsilon\sqrt{n}}$. Comparing the results of Theorems 4.3 and 4.5, under the constraints of Theorem 4.5 we obtain that

$$\sum_{j=1}^{k} \lambda_j \le \nu_k(H) \le q^2 \sum_{j=1}^{k} \lambda_j, \quad \text{where} \quad 1 < q < 2.$$

This means, that provided ε is less than $\dfrac{1}{2\sqrt{n}}$, then q is at most 2, and the combinatorial and analytical measures of H, $\nu_k(H)$ and $\sum_{j=1}^{k} \lambda_j$ differ at most by a factor of 4.

5. Optimal Partitions of Weighted Graphs

Similar statements can be proved for the spectrum of a weighted graph $G = (V, \mathbf{W})$. Here more precise perturbation results for the representatives are examined. We shall need a definition.

DEFINITION 5.1 *The k-variance of the vectors $\mathbf{x}_1, \dots, \mathbf{x}_n \in R^{k-1}$ with respect to the k-partition P_k is defined by*

$$S_k^2(P_k, \mathbf{X}) := \sum_{i=1}^{k} \sum_{j:c(j)=i} \left\| \mathbf{x}_j - \frac{\sum_{l:c(l)=i} \mathbf{x}_l}{n_i} \right\|^2,$$

where $n_i = |V_i|$. The k-variance of the vectors $\mathbf{x}_1, \dots, \mathbf{x}_n$ is defined by

$$S_k^2(\mathbf{X}) := \min_{P_k \in \mathcal{P}_k} S_k^2(P_k, \mathbf{X}).$$

Even if no a well-separated k-partition of the optimal $(k-1)$-dimensional representatives $\mathbf{x}_1^*, \dots, \mathbf{x}_n^*$ exists, it can be asked how the k-variance $S_k^2(\mathbf{X}^*)$ of them depends on the eigenvalues. To get some perturbation results, the following situation is investigated:

Let P_k be a fixed k-partition of the set of vertices (sometimes we shall refer to it as a colouring). The Laplacian $\mathbb{C}$ of the weighted graph G can be decomposed as $\mathbb{B} + \mathbb{P}$, where $\mathbb{P}$ is the Laplacian of the weighted graph formed from G by retaining the bicoloured edges with respect to the colouring P_k, while $\mathbb{B}$ is the Laplacian of the weighted graph obtained by retaining the monocoloured ones. The matrix $\mathbb{B}$ has the eigenvalue 0 with multiplicity k, the corresponding eigenspace can be spanned by k pairwise orthogonal vectors (let us denote them by $\mathbf{u}_1, \dots, \mathbf{u}_k$) so that all the coordinates of the l^{th} vector – being different from those assigned to the vertices of V_l – are equal to 0, $(l = 1, \dots, k)$. Let us denote by ϱ the smallest positive eigenvalue of the matrix $\mathbb{B}$. It is the minimum of the smallest positive eigenvalues of the weighted sub-graphs induced by the vertices of the parts V_i-s of the k-partition P_k. Put $\varepsilon := \|\mathbb{P}\|$ and suppose that $\varepsilon < \varrho$. THEOREM 5.2 *Under the above assumptions*

$$S_k^2(P_k, \mathbf{X}^*) \le k \frac{\varepsilon}{\varrho}$$

holds for the k-variance of the optimal $(k-1)$-dimensional representatives $\mathbf{x}_1^*, \dots, \mathbf{x}_n^*$. We remark that

$$\varepsilon = \|\mathbb{P}\| \le \operatorname{tr} \mathbb{P} = \sum_{\substack{i,j \\ c(i) \ne c(j)}} w_{ij} = v(P_k)$$

and

$$\varrho = \min_i \lambda_1(\mathbb{B}_i) \ge \begin{cases} 2(1 - \cos \frac{\pi}{n_i})\mu_2(G_i), & \text{if } 0 \le \mu_2(G_i) \le \frac{1}{2} d_{i\max} \\ c_{i1}\mu_2(G_i) - c_{i2} d_{i\max}, & \text{if } \frac{1}{2} d_{i\max} < \mu_2(G_i), \end{cases}$$

where $c_{i1} = 2(\cos \frac{\pi}{n_i} - \cos \frac{2\pi}{n_i})$, $c_{i2} = 2 \cos \frac{\pi}{n_i}(1 - \cos \frac{\pi}{n_i})$, $d_{i\max} = \max_{j \in V_i} d_j$ – see FIEDLER (1973) – and $\mathbb{B}_i$ is the Laplacian of the induced weighted subgraph G_i by the vertex set V_i (on n_i vertices). $\mathbb{B}_i$ is just the i^{th} diagonal block of $\mathbb{B}$. Therefore the 'smaller' the volume of the k-partition P_k and the greater the 2-cut of the monocoloured ones is (this means that the G_i-s are strongly connected), the better the optimal k-dimensional representatives of the vertices can be classified into k clusters. This reasoning also gives us some idea on the choice of the k-partition P_k. The next proposition estimates the k-variance of the optimal k-partition.

PROPOSITION 5.3 *Let $\mathbf{X}^*$ be an optimal $(k-1)$-dimensional representation of the above weighted graph. Then for the k-variance of the optimal $(k-1)$-dimensional representatives*

$$S_k^2(\mathbf{X}^*) \le S_k^2(P_k, \mathbf{X}^*) \le \frac{\lambda_1 + \cdots + \lambda_{k-1}}{\varrho(P_k)}$$

holds with any k-partition P_k. Notice that the more 'concise' the edges within the G_i-s are, the greater $\varrho(P_k)$ is.

The question naturally arises: does in general the existence of a gap in the spectrum between λ_{k-1} and λ_k itself result in a 'small' $(k-1)$-variance of the optimal k-dimensional representatives? This is answered, at least partly, in the next section.

6. Gaps in the Spectrum of a Weighted Graph

Let $G = (V, \mathbf{W})$ be a weighted graph with weight matrix $\mathbf{W}$ of the edges and $\mathbf{D} = \mathrm{diag}(d_1, \ldots, d_n)$ of the vertices, where $d_i = \sum_{j \ne i} w_{ij}$, $(i = 1, \ldots, n)$. Suppose that $\sum\limits_{i=1}^{n} \sum\limits_{j=1}^{n} w_{ij} = 1$. According to Section 3 the spectrum of this weighted graph is defined by the eigenvalues of the weighted Laplacian $\mathbf{C}_D$.

THEOREM 6.1 *Let $0 = \lambda_0 < \lambda_1 < \lambda_2 \le \cdots \le \lambda_{n-1}$ denote the eigenvalues of the weighted Laplacian $\mathbf{C}_D$ and let $\mathbf{X}^*$ be the optimal 1-dimensional representation of the vertices (it is just the eigenvector corresponding to λ_1). Then*

$$S_2^2(\mathbf{X}^*) \le \frac{\lambda_1}{\lambda_2}.$$

The theorem implies the following expanding property of the eigenvalues: the greater the gap between the two smallest positive eigenvalues of G is, the better the optimal 1-dimensional representatives of the vertices can be classified into two clusters.

For establishing similar relations between the $(k+1)$-variance of an optimal k-dimensional representation of the vertices of the above weighted graph and the gap of the spectrum of its weighted Laplacian $\mathbf{C}_D$ between the eigenvalues λ_k and λ_{k+1} we would like to prove the following conjecture:

CONJECTURE 6.2 *Let $0 = \lambda_0 \le \lambda_1 \le \cdots \le \lambda_k < \lambda_{k+1} \le \cdots \le \lambda_{n-1}$ be the spectrum of the weighted Laplacian $\mathbf{C}_D = \mathbf{I}_n - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$ of the weighted graph G with weight matrix $\mathbf{W}$, where $\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} = 1$, $d_i = \sum_{\substack{j=1 \\ j \ne i}}^{n} w_{ij}$ and $\mathbf{D} = diag(d_1, \ldots, d_n)$. Let $\mathbf{x}_1^*, \ldots, \mathbf{x}_n^* \in R^k$ be optimal k-dimensional representatives of the vertices satisfying the conditions*

$\sum_{i=1}^n d_i \mathbf{x}_i^* = 0$ and $\sum_{i=1}^n d_i \mathbf{x}_i^* \mathbf{x}_i^{*T} = \mathbf{I}_k$. Let $S_{k+1}^2(\mathbf{x}_1^*, \dots, \mathbf{x}_n^*)$ denote the $(k+1)$-variance of the vectors $\mathbf{x}_1^*, \dots, \mathbf{x}_n^*$. Then

$$S_{k+1}^2(\mathbf{x}_1^*, \dots \mathbf{x}_n^*) \le k \cdot \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_{k+1}}, \qquad 1 \le k < n-1.$$

For the proof we would need the following LEMMA 6.3 There exists a transformation $y_i = f(\mathbf{x}_i^*)$ so that the function f satisfies the Lipschitz condition, $\sum_{i=1}^n d_i y_i = 0$, $\sum_{i=1}^n d_i \mathbf{x}_i^* y_i = 0$ and $\sigma^2(\mathbf{y}) := \sum_{i=1}^n d_i y_i^2 \ge S_{k+1}^2(\mathbf{x}_1^*, \dots, \mathbf{x}_n^*)$. Our conjecture is that with Lipschitz constant $\sqrt{k}$ such an y can be found. For some special representations even we have a construction, but in general it is not sure that such construction exists at all.

This means that supposing the optimal k-dimensional representatives form $k+1$ well-separated clusters and there is a gap in the spectrum between the eigenvalues λ_k and λ_{k+1}, then the $(k+1)$-variance of the optimal k-dimensional representatives $\mathbf{x}_1^*, \dots, \mathbf{x}_n^*$ can be estimated from above by this gap. But a construction can be given that the $(k+1)$-variance is small, however, this gap does not occur. (This is because the eigenvalues do not determine the eigenvectors and vice versa.) Nevertheless, the spectrum can give us some idea about the number of clusters. But a sufficient condition and the classification itself can be obtained only by means of Euclidean representations.

7. Some Remarks Concerning Spectra of Multigraphs

Finally, we introduce some simple propositions on spectra of hypergraphs and on Euclidean representations of some special hypergraphs (sometimes without proofs). Unless otherwise stated, the propositions refer to the spectral characteristics of the hypergraph $H = (V, E)$ with $|V| = n$ and $|E| = m$.

ASSERTION 7.1 If $H_i = (V, E_i)$, $(i = 1, \dots, k)$ are edge-disjoint hypergraphs, and $H = (V, E)$, where $E = \cup_{i=1}^k E_i$, $E_i \cap E_j = \emptyset$ $(i \ne j)$, then for their connectivity matrices the relation

$$\mathbf{B}(H) = \sum_{i=1}^k \mathbf{B}(H_i) \tag{7.1}$$

holds. □ PROPOSITION 7.2 Let $H = (V, E)$ be a hypergraph, $E = E_1 \cup E_2$, $E_1 \cap E_2 = \emptyset$, $H_i = (V, E_i)$, $i = 1, 2$. Then

$$\sum_{j=1}^k \lambda_j \ge \sum_{j=1}^k \lambda_j^{(1)} + \sum_{j=1}^k \lambda_j^{(2)}, \quad (1 \le k \le n), \tag{7.2}$$

where $\lambda_j^{(i)}$ denotes the j-th eigenvalue of H_i in increasing order $(i = 1, 2)$. PROPOSITION 7.3 With the notations of the previous proposition:

$$\lambda_{j-r_i} \leq \lambda_j^{(i)} \leq \lambda_j, \quad (j = 1, \dots, n), \tag{7.3}$$

where $r_i = \operatorname{rank} \mathbb{B}_i$, $\mathbb{B}_i$ being the connectivity matrix of H_i $(i = 1, 2)$ and $\lambda_l = 0$, if $l < 1$. COROLLARY 7.4 For $z = 2$, by the successive and alternating application of the two sides of (7.3) we obtain that

$$0 \leq \lambda_2' \leq \lambda_2 \leq \lambda_2' + \lambda_3' \leq \lambda_2 + \lambda_3 \leq \lambda_2' + \lambda_3' + \lambda_4' \leq \lambda_2 + \lambda_3 + \lambda_4 \leq \cdots . \quad \square \tag{7.4}$$

EXAMPLE 7.5 Let C_n denote the complete hypergraph with n vertices and without loops (it has $2^n - n - 1$ hyperedges). Its spectrum consists of one zero and the number $\dfrac{n2^{n-1} - 2^n + 1}{n-1}$ with multiplicity $n - 1$. Any $n - 1$ pairwise orthogonal vectors within the subspace orthogonal to the vector $\mathbb{e} \in R^n$ are eigenvectors belonging to the multiple eigenvalue. $\square$EXAMPLE 7.6 The smallest positive eigenvalue of the path graph P_n having $n = 2l+1$ vertices is $1 - \cos\frac{\pi}{n}$. Labelling the vertices as $v_{-l}, \dots, v_0, \dots, v_l$, the second coordinates of their representatives in the optimal 2-dimensional Euclidean representation of P_n are

$$x_j = \frac{\sqrt{2}}{\sqrt{n}} \sin(j\frac{\pi}{n}), \quad j = -l, \dots, 0, \dots, l \tag{7.5}$$

while the first coordinates are all equal to $\frac{1}{\sqrt{n}}$. $\square$

EXAMPLE 7.7 Let S_d denote the star graph with $n = d + 1$ vertices. The smallest positive eigenvalue of S_d is $1/2$ with multiplicity $d - 1$. An optimal d-dimensional Euclidean representation of S_d is a d-simplex in the $(d-1)$-dimensional subspace of R^d orthogonal to the vector $\mathbb{e} \in R^d$. The centre of gravity of the simplex is in the origin. The representatives of the vertices of valency 1 are the vertices, while the representative of the vertex of valency d is the centre of gravity of the simplex. $\square$

EXAMPLE 7.8 Let $G_{d,l}$ denote the subdivision graph of S_d, where each of the edges of S_d is divided into l parts. We call $G_{d,l}$ spider with d feet and l sections. The number of its vertices is $n = dl + 1$. The smallest positive eigenvalue of $G_{d,l}$ is of multiplicity $d - 1$ and it is equal to $1 - \cos\frac{\pi}{2l+1}$. An optimal d-dimensional Euclidean representation of the spider $G_{d,l}$ is obtained from those of S_d and P_{2l+1}, where the feet of the spider are divided according to the sine rhythm of (7.9). $\square$

EXAMPLE 7.9 Let $L_{d,l}$ denote the d-dimensional lattice whose vertices are all d-tuples of numbers $-l, \dots, 0, \dots, l$, where two d-tuples are adjacent if and only if they differ in exactly one coordinate. The number of its vertices is $n = (2l+1)^d$. The smallest positive eigenvalue of $L_{d,l}$ is $1 - \cos\frac{\pi}{2l+1}$ with multiplicity d. An optimal $(d+1)$-dimensional Euclidean representation of $L_{d,l}$ is realized in the d-dimensional subspace of R^{d+1} orthogonal to the $\mathbf{e} \in R^{d+1}$ vector. It is a d-dimensional lattice, its centre of gravity being in the origin, and the distances between the representatives of adjacent vertices follow the sine rhythm of (7.9). □

EXAMPLE 7.10 Let $K_{n_1,\dots,n_k}$ be the complete k-partite graph, where $n = \sum_{i=1}^{k} n_i$ (n being the number of vertices). Let $(V_1,\dots,V_k)$ denote the colour classes where $|V_i| = n_i$, $(i = 1,\dots,k)$. The spectrum of $K_{n_1,\dots,n_k}$ contains a single 0, the numbers $\frac{1}{2}(n-n_i)$ with multiplicity $n_i - 1$ $(i = 1,\dots,k)$ and $k-1$ numbers are equal to $\frac{1}{2}n$. If we regard the $(k-1)$-dimensional Euclidean representation corresponding to the largest eigenvalue $\frac{1}{2}n$, the representatives of the vertices in this representation constitute k different points in the $(k-1)$-dimensional Euclidean space, where the representatives of vertices of the same colour coincide.

In this way we can characterize the complete k-partite graph on the basis of its optimal $(k-1)$-dimensional Euclidean representation belonging to the largest eigenvalue with multiplicity $k-1$. But how we can recognize a k-colourable graph in a similar way, we do not know exactly. Recently it has turned out that these spectral techniques are not always capable of the recognition of the chromatic number.

Analogously to the derivation of the Representation Theorem the maximum of the quadratic form $L(\mathbb{X}) = \operatorname{tr} \mathbb{X}\mathbb{B}\mathbb{X}^T$ on $\mathbb{X}\mathbb{X}^T = \mathbb{I}_k$ is the sum of the k largest eigenvalues of the hypergraph in question and the $k \times n$ matrix $\mathbb{X}$ giving the maximum contains the corresponding eigenvectors in its rows. In this kind of representation the sum of the variances of edges is maximized. As a k-colourable graph has no edges within the subsets of colour-partition $(V_1,\dots,V_k)$, the $(k-1)$-dimensional representatives of vertices of the same colour tend to be near to each other, while the representatives of vertices of the multi-coloured edges tend to be far away. Consequently, the colour-partition frequently results in well-separated clusters of the representatives of vertices in this representation.

8. A Heuristic Classification Algorithm Based on Euclidean Representations

Let $v_1, v_2, \dots, v_n$ be binary random variables taking the values 0–1 and $e_1, e_2, \dots, e_m$ be a sample for them $(n \ll m)$. They form a hypergraph $H = (V, E)$ with vertex-set $V = \{v_1, v_2, \dots, v_n\}$ and edge-set

$E = \{e_1, e_2, \dots, e_m\}$, where $\mathcal{I}(v \in e) = v(e)$, $v(e)$ being the observed value of the variable v on the object e. (When v represents some property, $v(e) = 1$ means the presence, while $v(e) = 0$ the absence of this property on the object e.)

Let $E' \subset E$ be a *sub-sample.* The sub-hypergraph $H' = (V, E')$ is called the *hypergraph of the edge-cluster* E'. Let us denote by $0 = \lambda_1(H') \leq \lambda_2(H') \leq \dots \leq \lambda_n(H')$ the spectrum of H', while the $n \times n$ matrix $\mathbb{X}^*(H')$ contains a whole system of pairwise orthonormal eigenvectors of the connectivity matrix of H'. According to the Representation Theorem of Section 2, for any integer d $(1 \leq d \leq n)$ the $d \times n$ matrix $\mathbb{X}_d^*(H')$ — obtained from $\mathbb{X}^*(H')$ by retaining the eigenvectors corresponding to $\lambda_1(H'), \lambda_2(H') \dots, \lambda_d(H')$ — determines an optimal d-dimensional Euclidean representation of H'. Furthermore, the sum of the variances of edges of E' in this representation is minimal, and it is equal to

$$L(\mathbb{X}_d^*(H')) = \sum_{e \in E'} L(e, \mathbb{X}_d^*(H')) = \sum_{j=1}^{d} \lambda_j(H').$$

Put $K(H') := \min_{d=1}^{n} [c2^{n-d} + L(\mathbb{X}_d^*(H'))]$, where $c > 0$ is a constant (chosen previously according to the size of problem). The dimension d^* giving the minimum is called the *dimension of the edge-cluster* E'.

Let $\mathcal{S}$ denote the set of all partitions of E into non-empty disjoint sub-samples. Our purpose is to find a partition $S \in \mathcal{S}$ consisting of sub-samples E_i-s for which the objective function $K = \sum_i K(H_i)$ is minimal, where $H_i = (V, E_i)$ is the hypergraph belonging to the edge-cluster E_i.

Now let k be a fixed integer, $(1 \leq k \leq n)$. We shall define a numerical algorithm converging to a local minimum of the objective function, when the minimization takes place over the set of all k-partitions $\mathcal{S}_k$. Let $(E_1, \dots, E_k) \in \mathcal{S}_k$ be a k-partition of the edge-set of H. Applying the previous notations for the hypergraphs $H_i = (V, E_i)$, $(i = 1, \dots, k)$ the following cost function is constructed: $Q = \sum_{i=1}^{k} Q_{d_i}(H_i)$, where

$$Q_{d_i}(H_i) := c2^{n-d_i} + L(\mathbb{X}_{d_i}^*(H_i)), \quad (i = 1, \dots, k).$$

To minimize the cost function Q — with respect to k-partitions of the edges and dimensions of the edge-clusters — the following iteration is introduced. First let us choose k disjoint clusters $E_1, \dots, E_k$ of the objects (e.g. by the k-means method, see in [19]).

i. Fixing the clusters $E_1, \dots, E_k$: the spectra and optimal Euclidean representations of the sub-hypergraphs of the edge-clusters are calculated.

ii. The function $Q_{d_i}(H_i)$ is minimized with respect to the dimension d_i, $(1 \leq d_i \leq n)$ for each i separately. A unique d_i^* giving the i-th minimum always exists. As for it

$$Q_{d_i^*}(H_i) = c2^{n-d_i^*} + \sum_{j=1}^{d_i^*} \lambda_j(H_i) \quad (i = 1, \dots, k)$$

holds, in this step the cost function Q is decreased. Until this moment the minimization took place within the clusters. In the next step the objects are relocated between the clusters:

iii. Fixing the d_i^*-dimensional optimal Euclidean representations $\mathbf{X}_{d_i^*}^*(H_i)$-s: an object e is replaced into the cluster E_i, for which $L(e, \mathbf{X}_{d_i^*}^*(H_i))$ is minimal. If the minimum is taken for more than one i, let us replace e into the cluster E_i with the smallest index i. In this step Q is also decreased. In this way a new disjoint classification $E_1^*, \dots, E_k^*$ of the objects is obtained. From now on we go back to step i. with starting classification $E_1^*, \dots, E_k^*$, etc.

As the cost function Q is decreased in each step and in steps ii. and iii. discrete minimizations are performed, the algorithm must converge to a local minimum of Q in finite steps. It is easy to see that for fixed k the k-partition to which the iteration converges gives a local minimum of the objective function K, too. As a new step of the iteration, a minimization with respect to k could be introduced, but it would be very time-demanding. (The optimal value of k also depends on the constant c.)

During the iteration some edge-clusters may become empty. Also the hypergraph $H_i = (V, E_i)$ may contain isolated vertices (this results in additional zero eigenvalues). Let us denote by V_i the set of the non-isolated vertices of H_i. Provided H has no isolated vertices, then $\cup_{i=1}^k V_i = V$ and $V_1, \dots, V_k$ are not necessarily disjoint subsets of the vertices. V_i is called the *characteristic property-association* of the sub-sample E_i.

9. Summary

For the time being we have investigated Laplacian spectra and Euclidean representations of multigraphs merely in connection with the above classification property. The authors think that these spectral techniques are worth for further investigation because of the following reasons:

- In the case of large multigraphs (up to 100 vertices and arbitrary number of edges) there are numerical algorithms which can quickly perform the spectral characteristics.

- In low dimensions (mainly in 3 dimensions) and on special fields (e.g. in chemistry) relative location of the representatives of vertices realizes real spatial arrangement of certain atoms.
- The objective function Q itself has a physical meaning: It gives the variance of the whole system which is to be minimized on certain constraints.

The Hückel's theory – see CVETKOVIĆ (1979) – introduces a model of quantum theory where the stationary state of atoms can be obtained via the Schrödinger equation (it also contains the Laplacian operator). Describing the structure of the atoms the eigenvalues can be represented in special cases as energy levels of the electrons (called atomic orbitals).

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