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Spectra and optimal partitions of weighted graphs*

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Abstract

The notion of the Laplacian of weighted graphs will be introduced, the eigenvectors belonging to k consecutive eigen-values of which define optimal k-dimensional Euclidean representation of the vertices. By means of these spectral techniques some combinatorial problems concerning minimal $(k+1)$-cuts of weighted graphs can be handled easily with linear algebraic tools. (Here 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 eigen-values and by the gap in the spectrum between the kth and $(k+1)$th positive eigenvalues in increasing order.

1. Basic notations

Let $G=(V, W)$ be a weighted undirected graph, where $V:=\{v_1, \ldots, v_n\}$ is the set of its vertices and W is the *weight matrix* of the edges. The diagonal entries of the $n \times n$ matrix W are zero, while the nondiagonal entry w_{ij} is the weight assigned to the edge $\{v_i, v_j\}$ and $w_{ij}=w_{ji} \geqslant 0$, $i \neq j$. (If the vertices v_i and v_j are not adjacent, the weight w_{ij} is zero.) 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 $D=\operatorname{diag}(d_1, \ldots, d_n)$ be the diagonal matrix with d_j's in its main diagonal.

We would like to characterize some structural properties of weighted graphs by means of their spectra and Euclidean representations, as follows. Let k $(1 \leqslant k \leqslant n-1)$ be a fixed integer and let the vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in R^k$ satisfy the constraints $\sum_{j=1}^{n} \boldsymbol{x}_j \boldsymbol{x}_j^{\mathrm{T}} = \boldsymbol{I}_k$ and $\sum_{j=1}^{n} \boldsymbol{x}_j = \boldsymbol{0}$. The vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are regarded as k-dimensional

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representatives of the vertices. Let $X:=(x_1,\dots,x_n)$ be the $k\times n$ matrix containing the vectors x_j's as its columns. Let us define the quadratic form

$$Q:=\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|x_i-x_j\|^2=\operatorname{tr} XCX^{\mathrm T}, \tag{1.1}$$

where the $n\times n$ matrix C is equal to $D-W$. C is symmetric, singular and positive semidefinite. We call it the *Laplacian* of the weighted graph G, while Q is called the *quadratic form* belonging to G.

Let us denote by

$$0=\lambda_0\leqslant\lambda_1\leqslant\dots\leqslant\lambda_{n-1}$$

the eigenvalues of the Laplacian C. In [4] the following Representation Theorem is proved: the minimum of Q constrained on $XX^{\mathrm T}=I_k$ and $\sum_{j=1}^n x_j=0$ is $\sum_{j=1}^k\lambda_j$ and it is attained for $X^*=(u_1,\dots,u_k)^{\mathrm T}$, where $u_1,\dots,u_k\in R^n$ are k pairwise orthonormal eigenvectors corresponding to the eigenvalues $\lambda_1,\dots,\lambda_k$ of the matrix C. The column vectors $x_1^*,\dots,x_n^*$ of any optimal 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.

In [4] the problem is formulated in terms of hypergraphs, but a weighted graph can always be assigned to a hypergraph. Given a hypergraph $H=(V,E)$ the entries of the weight matrix W are the following:

$$w_{ij}=w_{ji}=\sum_{e\in E}\mathscr{I}(v_i\in e)\mathscr{I}(v_j\in e)\frac{1}{|e|}\quad(1\leqslant i<j\leqslant n),$$

where $|e|$ stands for the number of vertices contained by the hyperedge e and $\mathscr{I}(v\in e)$ equals to 1 or 0 depending on whether the hyperedge e contains the vertex v or not.

It is well-known that the multiplicity of the zero as an eigenvalue of the Laplacian is equal to the number of connected components of G. Therefore, in the sequel only connected weighted graphs are investigated.

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 W of the edges, the vertex v_j of which has the weight s_j $(j=1,\dots,n)$ and $S:=\operatorname{diag}(s_1,\dots,s_n)$. Now the quadratic form Q of (1.1) is minimized subject to the constraints that $\sum_{j=1}^n s_jx_jx_j^{\mathrm T}=XSX^{\mathrm T}=I_k$ and $\sum_{j=1}^n s_jx_j=0$. Since Q can be written as

$$\operatorname{tr} XCX^{\mathrm T}=\operatorname{tr}(XS^{1/2})[S^{-1/2}CS^{-1/2}](XS^{1/2})^{\mathrm T}, \tag{1.2}$$

the minimum of Q on the above constraint is $\sum_{j=1}^k\kappa_j$ — where $0=\kappa_0\leqslant\kappa_1\leqslant\dots\leqslant\kappa_{n-1}$ are the eigenvalues of the symmetric, singular, positive semidefinite matrix in brackets — and it is attained for the representation $X^*=(u_1,\dots,u_k)^{\mathrm T}S^{-1/2}$ of the vertices, where $u_1,\dots,u_k$ are k pairwise orthonormal eigenvectors corresponding to the k smallest positive eigenvalues of the so-called *weighted Laplacian* $C_S:=S^{-1/2}CS^{-1/2}$. With other words the $k\times n$ matrix $(\sqrt{s_1}x_1^*,\dots,\sqrt{s_n}x_n^*)$ — where the column vectors $x_1^*,\dots,x_n^*$ of any optimal X^* are called optimal k-dimensional representatives of the vertices — contains the above eigenvectors $u_1,\dots,u_k$ in its rows.

If the weight matrix S is equal to D, then the matrix C_D is equal to $I_n-D^{-1/2}WD^{-1/2}$. Let us denote by ϱ_i's the eigenvalues of the matrix $D^{-1/2}WD^{-1/2}$. Since for all i the relation $-1\leqslant\varrho_i\leqslant1$ holds, any eigenvalue $\kappa_i=1-\varrho_{n-i-1}$ of C_D is nonnegative and it is at most 2 $(i=0,\dots,n-1)$.

We remark that the graph G can be regarded as the product of two copies of the probability space $(I,\mathscr{A},P)$, $I=\{1,\dots,n\}$, $P=\{p_1,\dots,p_n\}$, where $p_i=d_i/\sum_{j=1}^n d_j$ and W can be normed in such a way that it is a symmetric measure on G. In this case $D^{-1/2}WD^{-1/2}$ defines the operator taking the conditional expectation between the two probability spaces and ϱ's are like canonical correlations.

2. Consistent colorings

Let $G=(V,W)$ be a weighted graph, and let k be a fixed integer $(1<k<n)$. Let $P_k=(V_1,\dots,V_k)$ denote a *k-partition* of the set of vertices and c_{P_k} denote the clustering (sometimes we shall refer to it as a coloring) defined by P_k in the following way: $c_{P_k}(j):=i$, if $v_j\in V_i$.

Definition 2.1. The vector $u\in R^n$, $\sum_{j=1}^n u(j)=0$ is called to be *P_k-consistent*, if it is constant on the parts of the k-partition P_k, i.e. $u(i)=u(j)$ whenever $c_{P_k}(i)=c_{P_k}(j)$, where $u(i)$ denotes the ith coordinate of the vector u.

Definition 2.2. The vertices of the weighted graph G are said to be *consistently k-colorable*, if there exists a k-partition P_k such that every P_k-consistent vector is an eigenvector of the Laplacian C of G.

It is easy to see that the P_k-consistent vectors for a given k-partition P_k constitute a $(k-1)$-dimensional subspace in R^n and if G is consistently k-colorable with respect to P_k, then the $(k-1)$-dimensional subspace spanned by the P_k-consistent eigenvectors is an eigenspace of the Laplacian C belonging to an eigenvalue λ with multiplicity $k-1$.

Theorem 2.3. *Let us fix the k-partition P_k. G is consistently k-colorable with respect to the k-partition P_k if and only if there exists a constant κ such that for all $i\in\{1,2,\dots,n\}$ and for each $p\neq c_{P_k}(i)$*

$$\sum_{j:\,v_j\in V_p} w_{ij}=\kappa n_p, \tag{2.1}$$

where $n_p=|V_p|$.

In the special case when W is the ordinary adjacency matrix, our theorem means that for every vertex v_i and for each color p (which is different from the color of v_i):

$$\sum_{j:\,v_j\in V_p} w_{ij}=\#\{e\colon e=\{v_i,v_j\},\ v_j\in V_p\}=\kappa n_p$$

holds, i.e. the number of edges connecting v_i with vertices of color p is proportional to the size of V_p and the coefficient of proportionality (κ) is the same for all i and $p \neq c_{P_k}(i)$.

Proof of Theorem 2.3. Let us fix the k-partition P_k. In the sequel we indicate P_k in a coloring only if P_k is different from the underlying k-partition.

Sufficiency: Suppose that there exists a constant κ such that for each integer $i \in \{1, \dots, n\}$ and $p \neq c(i)$ the relation

$$\sum_{j:\, v_j \in V_p} w_{ij} = \kappa n_p$$

holds. Let the vector $\boldsymbol{u} \in R^n$ be P_k-consistent and put $y_p := u(j)$, if $c(j) = p$. If $c(i) = l$, then the ith coordinate of the vector $\boldsymbol{Cu}$ is the following:

$$\left[\sum_{j:\, j \neq i} w_{ij} - \sum_{j:\, c(j) = l} w_{ij} \right] y_l - \sum_{\substack{p=1 \\ p \neq l}}^{k} \sum_{j:\, c(j) = p} w_{ij} y_p$$

$$= \kappa y_l \sum_{\substack{p=1 \\ p \neq l}}^{k} n_p - \kappa \sum_{\substack{p=1 \\ p \neq l}}^{k} n_p y_p = \kappa n y_l,$$

because $\sum_{p=1}^{k} n_p y_p = 0$. Therefore, $\boldsymbol{u}$ is an eigenvector of the Laplacian C with corresponding eigenvalue $n\kappa$.

Necessity: Let $\boldsymbol{u}$ be a P_k-consistent eigenvector of the Laplacian C. Then there exists an eigenvalue λ with multiplicity $k-1$ for which

$$\boldsymbol{Cu} = \lambda \boldsymbol{u}, \tag{2.2}$$

and there are real numbers $y_1, \dots, y_k$ such that $\sum_{i=1}^{k} n_i y_i = 0$ and $u(j) = y_i$, if $c_{P_k}(j) = i$. Let us fix the integer l. Let us choose an index i such that $c(i) = l$. Let us introduce the following notations:

$$s_i := \sum_{j:\, j \neq i} w_{ij} \quad \text{and} \quad s_{ip} := \sum_{j:\, c(j) = p} w_{ij}.$$

With these notations, the equation (2.2) for the ith coordinate of the vector $\boldsymbol{Cu}$ gives

$$(s_i - s_{il}) y_l - \sum_{\substack{p=1 \\ p \neq l}}^{k} s_{ip} y_p = \lambda y_l,$$

whence

$$\left(\sum_{\substack{p=1 \\ p \neq l}}^{k} s_{ip} - \lambda \right) y_l = \sum_{\substack{p=1 \\ p \neq l}}^{k} s_{ip} y_p. \tag{2.3}$$

We remark that the equation does not depend on the weights w_{ij}'s for which $c(j) = l$. With the notation

$$z_{ip} := \begin{cases} \lambda - \sum_{\substack{q=1 \\ q \neq p}}^{k} s_{iq} & \text{if } p = l, \\ s_{ip} & \text{if } p \neq l \end{cases} \tag{2.4}$$

equation (2.3) becomes

$$\sum_{p=1}^{k} z_{ip} y_p = 0,$$

and this holds for every k-tuples $y_1, \dots, y_k$ of real numbers such that $\sum_{p=1}^{k} n_p y_p = 0$. Therefore, for each index i there must exist a constant κ_i such that $z_{ip} = \kappa_i n_p$, $(p = 1, \dots, k)$. Substituting it into (2.4) for $p \neq l$ one obtains that $s_{ip} = \kappa_i n_p$, whence

$$\sum_{\substack{q=1 \\ q \neq l}}^{k} s_{iq} = \kappa_i \sum_{\substack{q=1 \\ q \neq l}}^{k} n_q = \kappa_i (n - n_l).$$

Again substituting it into (2.4) for $p = l$ we arrive at $\kappa_i n_l = z_{il} = \lambda - \kappa_i (n - n_l)$, whence $\lambda = \kappa_i n$. Therefore, κ_i — consequently s_{ip} — does not depend on i and there exists a constant κ — namely $\kappa = \lambda / n$ — such that for each $p \neq c(i)$ the equation $\sum_{v_j \in V_p} w_{ij} = \kappa n_p$ holds. □

We have also proved that $\kappa = \lambda / n$, where λ is the eigenvalue with multiplicity $k-1$ belonging to the $(k-1)$-dimensional eigenspace spanned by the P_k-consistent eigenvectors.

Since s_{ip} does not depend on i, hereby we shall denote it by s_p. In this way for any P_k-consistent vector $\boldsymbol{u}$

$$\lambda = \boldsymbol{u}^{\mathrm{T}} \boldsymbol{Cu} = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} (u(i) - u(j))^2$$

$$= \sum_{l=1}^{k-1} \sum_{m=l+1}^{k} \left[\sum_{i:\, c(i) = l} \sum_{j:\, c(j) = m} w_{ij} \right] (y_l - y_m)^2$$

$$= \sum_{l=1}^{k-1} \sum_{m=l+1}^{k} w'_{lm} (y_l - y_m)^2$$

holds, where w'_{lm} is the sum of the weights of the edges connecting the vertices of color l with those of color m. By an easy counting argument for $l \neq m$ the equation $w'_{lm} = \kappa n_l n_m = (\lambda / n) n_l n_m$ also holds.

In the case when G is consistently k-colorable with respect to some k-partition P_k, the corresponding multiple eigenvalue and the eigenspace of the P_k-consistent vectors can be obtained by the spectral decomposition of the following 'reduced' weighted graph G' on k vertices, the vertices of which are weighted too: the weight of the vertex

v'_l is n_l, while the weight of the edge $\{v'_l, v'_m\}$ is w'_{lm}. The entries of the Laplacian C' of G' are as follows:

$$c'_{lm} = \begin{cases} -\frac{\lambda}{n} n_l n_m & \text{if } l \neq m, \\ \lambda n_l - \frac{\lambda}{n} n_l^2 & \text{if } l = m. \end{cases}$$

Let us also introduce the following notations: $e \in R^k$ be the k-dimensional vector of 1's, $\boldsymbol{h} := (n_1, \ldots, n_k)^{\mathrm{T}}$, $\boldsymbol{S} := \mathrm{diag}(n_1, \ldots, n_k)$.

Let us denote by $\boldsymbol{u} \in R^n$ a P_k-consistent eigenvector of the weighted graph G with respect to the k-partition $P_k = (V_1, \ldots, V_k)$, $|V_i| = n_i$. Let λ denote the corresponding multiple eigenvalue. We have seen that the first n_1 coordinates of $\boldsymbol{u}$ are equal to y_1, the second n_2 ones to $y_2, \ldots$ while the last n_k ones to y_k, where $\sum_{i=1}^k n_i y_i = 0$.

Proposition 2.4. *Denoting by* $\boldsymbol{y}$ *the* k*-dimensional vector of coordinates* $y_1, \ldots, y_k$*, it is an eigenvector corresponding to the eigenvalue* λ *of the reduced weighted graph* G'*, the vertices of which are weighted with the weight matrix* $\boldsymbol{S} = \mathrm{diag}(n_1, \ldots, n_k)$.

Proof. With the above notations,

$$C' = -\frac{\lambda}{n} \boldsymbol{h}\boldsymbol{h}^{\mathrm{T}} + \lambda \boldsymbol{S} = \lambda \left(\boldsymbol{S} - \frac{1}{n} \boldsymbol{h}\boldsymbol{h}^{\mathrm{T}} \right)$$

$$= \lambda \boldsymbol{S}^{1/2} \left[\boldsymbol{I}_k - \left(\frac{\boldsymbol{S}^{-1/2}\boldsymbol{h}}{\sqrt{n}} \right) \left(\frac{\boldsymbol{S}^{-1/2}\boldsymbol{h}}{\sqrt{n}} \right)^{\mathrm{T}} \right] \boldsymbol{S}^{1/2}$$

holds. Let us denote the vector in parenthesis by $\boldsymbol{f}$, $\|\boldsymbol{f}\|^2 = 1$. The eigenvalues of the $k \times k$ matrix in brackets are one 0 with corresponding eigenvector $\boldsymbol{f}$ and the number 1 with multiplicity $k-1$, the corresponding eigenspace being orthogonal to the vector $\boldsymbol{f}$. Let $l < k$ be a fixed integer and $\boldsymbol{Y} = (\boldsymbol{y}_1, \ldots, \boldsymbol{y}_k)$ be an $l \times k$ matrix such that $\boldsymbol{Y}\boldsymbol{S}\boldsymbol{Y}^{\mathrm{T}} = \boldsymbol{I}_l$ and $\sum_{i=1}^k n_i \boldsymbol{y}_i = \boldsymbol{0}$. Then according to the Representation Theorem, the minimum of the quadratic form

$$\mathrm{tr}\, \boldsymbol{Y} C' \boldsymbol{Y}^{\mathrm{T}} = \lambda\, \mathrm{tr} (\boldsymbol{Y}\boldsymbol{S}^{1/2}) [\boldsymbol{I}_k - \boldsymbol{f}\boldsymbol{f}^{\mathrm{T}}] (\boldsymbol{Y}\boldsymbol{S}^{1/2})^{\mathrm{T}}$$

on the above constraints is $(l-1)\lambda$ and it is attained when the matrix $\boldsymbol{Y}\boldsymbol{S}^{1/2}$ contains l pairwise orthonormal eigenvectors of the matrix $\boldsymbol{I}_k - \boldsymbol{f}\boldsymbol{f}^{\mathrm{T}}$ corresponding to its l smallest positive eigenvalues. The columns of the matrix $\boldsymbol{Y}$ are the representatives of the vertices of the reduced graph G'.

Let us denote by $y_l(i)$ the ith coordinate of the representative of the lth vertex of G'. Then for any coordinate i the relation $\sum_{l=1}^k n_l y_l(i) = 0$ holds; therefore, any P_k-consistent eigenvector of the graph G can be obtained from the eigenvectors of the reduced weighted graph G' with the same eigenvalue. □

3. Optimal classifications

Our aim is to classify the vertices of the weighted graph $G = (V, W)$ in such a way that edges with large weights would connect possibly vertices of the same cluster. Some combinatorial measures characterizing this structural property are introduced and related to the spectral characteristics of G.

Let us fix the k-partition P_k and let us denote by c the clustering (coloring) belonging to it.

Definition 3.1. The *volume* $v(P_k)$ of the k-partition $P_k = (V_1, \ldots, V_k)$ is defined by

$$v(P_k) := \sum_{l=1}^{k-1} \sum_{m=l+1}^{k} w'_{lm}$$

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

$$u(P_k) := \sum_{l=1}^{k-1} \sum_{m=l+1}^{k} \left(\frac{1}{n_l} + \frac{1}{n_m} \right) w'_{lm},$$

where

$$w'_{lm} = \sum_{i:\, c(i)=l} \sum_{j:\, c(j)=m} w_{ij} \quad (1 \leq l < m \leq k) \quad \text{and} \quad n_p = |V_p|.$$

The *minimal k-cut* of the weighted graph G is defined by

$$\mu_k := \min_{P_k \in \mathscr{P}_k} v(P_k), \tag{3.1}$$

while the *minimal weighted k-cut* by

$$\nu_k := \min_{P_k \in \mathscr{P}_k} u(P_k), \tag{3.2}$$

where $\mathscr{P}_k$ denotes the set of all k-partitions of V.

Definition 3.2. The k-variance of the vectors $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in R^{k-1}$ with respect to the k-partition P_k is defined by

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

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

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

Definition 3.3. The cost of the edge $e = \{v_i, v_j\}$ $(i < j)$ with weight w_{ij} in the Euclidean representation $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ of the vertices is defined by $K(e) := w_{ij} \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$.

It is trivial that $\sum_{j=1}^k \lambda_j$ is the sum of the costs of the edges in an optimal $(k-1)$-dimensional Euclidean representation of the weighted graph G. In [4] it is proved that $\sum_{j=1}^k \lambda_j \leq \nu_{k+1}$ and if there exists a well-separated k-partition of the optimal $(k-1)$-dimensional representatives $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*$ of the vertices (the diameters of the clusters being $\varepsilon < 1/(2\sqrt{n})$, then $\nu_k \leq q^2 \sum_{j=1}^{k-1} \lambda_j$, where $q = 1 + \sqrt{n}\varepsilon/(1-\sqrt{n}\varepsilon)$. Therefore, the greater the gap between λ_{k-1} and λ_k is and the better the optimal $(k-1)$-dimensional representatives of the vertices can be classified into k clusters, the greater the difference between the combinatorial measures ν_k and ν_{k+1} is.

Even if there does not exist a well-separated k-partition of the optimal $(k-1)$-dimensional representatives $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*$, it can be asked, how the k-variance $S_k^2(X^*)$ of them depends on the eigenvalues. In order to get some perturbation results, the following two cases are investigated:

(i) The Laplacian $\boldsymbol{C}$ of the weighted graph G can be written as $\boldsymbol{B} + \boldsymbol{P}$, where $\boldsymbol{P}$ is the Laplacian of the weighted graph formed from G by retaining the bicolored edges with respect to the coloring P_k, while $\boldsymbol{B}$ is the Laplacian of the weighted graph obtained by retaining the monocolored ones. As the vertices of the latter weighted graph are consistently k-colorable with respect to the k-partition P_k and the matrix $\boldsymbol{B}$ has the eigenvalue 0 with multiplicity k, the corresponding eigenspace can be spanned by k pairwise P_k-consistent vectors (let us denote them by $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k$) such that all the coordinates of the lth vector — being different from those assigned to the vertices of V_l — are equal to 0 $(l = 1, \ldots, k)$. Such a matrix $\boldsymbol{B}$ is called to be 0-*ideal* (here the sum of the coordinates is not zero). Let us denote by ϱ the smallest positive eigenvalue of the 0-ideal matrix $\boldsymbol{B}$. It is the minimum of the smallest positive eigenvalues of the weighted subgraphs induced by the vertices of the parts V_i's of the k-partition P_k. Put $\varepsilon := \|\boldsymbol{P}\|$ and suppose that $\varepsilon < \varrho$.

(ii) Let the matrix $\boldsymbol{B}$ be the Laplacian of a weighted graph that is consistently k-colorable with respect to the k-partition P_k and the multiple eigenvalue $\lambda > 0$ is of multiplicity $k-1$. This $\boldsymbol{B}$ is called to be λ-*ideal*. Suppose that $\boldsymbol{B}$ has no more eigenvalues in the interval $(\lambda - \varrho, \lambda + \varrho)$. Put $\boldsymbol{P} := \boldsymbol{C} - \boldsymbol{B}$ and $\varepsilon := \|\boldsymbol{P}\|$. Suppose that $\varepsilon < \varrho$.

In the case (i) the $(k-1)$-dimensional representatives $\boldsymbol{x}_j$'s of the vertices are obtained from the eigenvectors corresponding to the $k-1$ smallest positive eigenvalues of the Laplacian $\boldsymbol{C}$, while in the case (ii) they are obtained from the eigenvectors corresponding to $k-1$ eigenvalues $\kappa_1, \ldots, \kappa_{k-1}$ 'near' to λ (the existence of such eigenvalues is guaranteed by Lemma 4.5).

In both cases let us denote by X the matrix formed from the above $(k-1)$-dimensional representatives $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ of the vertices as columns.

Furthermore, in case (ii) let us denote by $\chi_{k-1}(P_k)$ the sum of the costs of the edges in the $(k-1)$-dimensional Euclidean representation defined by $k-1$ pairwise orthonormal eigenvectors $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_{k-1}$ of $\boldsymbol{B}$ corresponding to the multiple eigenvalue λ (they are all consistent with P_k). Similarly, in case (i) let us denote by $\tau_k(P_k)$ the sum of the costs of the edges in the representation defined by k pairwise orthonormal eigenvectors $\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k$ of $\boldsymbol{B}$ corresponding to the eigenvalue 0 with multiplicity k. It is easy to see that $\tau_k(P_k) = u(P_k)$ (see [4], the proof of Theorem 3.5), where $P_k = (V_1, \ldots, V_k)$ is the k-partition being investigated. Therefore $\tau_k(P_k) \geq \sum_{j=1}^{k-1} \lambda_j$ holds trivially for all k-partition P_k, consequently $\nu_k \geq \sum_{j=1}^{k-1} \lambda_j$ is also valid.

With the above notations and assumptions the following theorems are proved. Let $X^* = (\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*)$ be an optimal $(k-1)$-dimensional Euclidean representation of the vertices of the weighted graph $G = (V, W)$, as it is discussed above (in case (ii) X^* contains $k-1$ pairwise orthogonal eigenvectors corresponding to the eigenvalues $\kappa_1, \ldots, \kappa_{k-1}$). Let P_k be the fixed k-partition.

Theorem 3.4. *Under assumptions* (i),

$$S_k^2(P_k, X^*) \leq k \frac{\varepsilon}{\varrho}, \tag{3.3}$$

while under assumptions (ii),

$$S_k^2(P_k, X^*) \leq (k-1) \frac{\varepsilon^2}{(\varrho - \varepsilon)^2} \tag{3.4}$$

holds for the k-variances of the optimal $(k-1)$*-dimensional representatives* $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*$.

We remark that

$$\varepsilon = \|\boldsymbol{P}\| \leq \operatorname{tr} \boldsymbol{P} = \sum_{\substack{i,j \\ c(i) \neq c(j)}} w_{ij} = v(P_k)$$

and

$$\varrho = \min_i \lambda_1(\boldsymbol{B}_i) \geq \begin{cases} 2(1-\cos(\pi/n_i)\mu_2(G_i) & \text{if } 0 \leq \mu_2(G_i) \leq \frac{1}{2} d_i^{\max} \\ c_{i1}\mu_2(G_i) - c_{i2} d_i^{\max} & \text{if } (1/2) d_i^{\max} < \mu_2(G_i), \end{cases}$$

where $c_{i1} = 2(\cos(\pi/n_i) - \cos(2\pi/n_i))$, $c_{i2} = 2\cos(\pi/n_i)(1-\cos(\pi/n_i))$, $d_i^{\max} = \max_{j \in V_i} d_j$ and $\boldsymbol{B}_i$ is the Laplacian of the induced weighted subgraph G_i by the vertex set V_i (on n_i vertices). $\boldsymbol{B}_i$ is just the ith diagonal block of $\boldsymbol{B}$ (see [3, Theorem 3.6]). Therefore, the 'smaller' the volume of the k-partition P_k and the greater the 2-cut of the monocolored 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.

For ordinary graphs this requirement means that there be 'few' bicolored edges and a lot of monocolored ones for possibly each color.

Theorem 3.5. *Under assumptions* (i),

$$\tau_k(P_k) - \sum_{j=1}^{k-1} \lambda_j \leq 2\varepsilon\sqrt{2}k \sqrt{\frac{\varepsilon}{\varrho}}, \tag{3.5}$$

while under assumptions (ii),

$$\chi_{k-1}(P_k) - \sum_{j=1}^{k-1} \kappa_j \leq (2\varepsilon + \lambda + \lambda_{n-1})\sqrt{2}(k-1)\frac{\varepsilon}{\varrho - \varepsilon} \tag{3.6}$$

holds for the differences between the sum of the costs of the edges and the sum of the eigenvalues, the eigenvectors corresponding to which define the representation, where λ_{n-1} *is the largest eigenvalue of the Laplacian* $\boldsymbol{C}$.

Proposition 3.6. *Let 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*

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

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: in general does 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 Section 5.

4. Proof of theorems

Lemma 4.1. *Let the $n \times n$ symmetric matrix $\boldsymbol{B}$ have the following property: there exists a k-dimensional subspace $F \subset R^n$ such that $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{Bx} \notin (a,b)$ for all $\boldsymbol{x} \in F$ ($\|\boldsymbol{x}\|=1$), where $a<b$ are real numbers ($a=-\infty$ or $b=\infty$ is allowed). Then $\boldsymbol{B}$ has at least k eigenvalues outside the interval (a,b).*

Proof. Let us denote by m the number of the eigenvalues of $\boldsymbol{B}$ inside the interval (a,b) and by H the subspace spanned by the corresponding eigenvectors. Then

$$k+m=\dim(F)+\dim(H)\leqslant n,$$

which finishes the proof, since the number of the eigenvalues of $\boldsymbol{B}$ outside (a,b) is equal to $n-m\geqslant k$. □

Corollary 4.2. *With the previous notations the following statements also hold:*

(a) *if there exists a k-dimensional subspace $F \subset R^n$ such that $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{Bx} \geqslant a$ for all $\boldsymbol{x}\in F$ ($\|\boldsymbol{x}\|=1$) — where a is a real number — then $\boldsymbol{B}$ has at least k eigenvalues that are at least a. (Hint: apply Lemma 4.1 with $b=\infty$.)*

(b) *if there exists a k-dimensional subspace $F \subset R^n$ such that $\boldsymbol{x}^{\mathrm{T}}\boldsymbol{Bx} \leqslant b$ for all $\boldsymbol{x}\in F$ ($\|\boldsymbol{x}\|=1$) — where b is a real number —, then $\boldsymbol{B}$ has at least k eigenvalues being at most b. (Hint: apply Lemma 4.1 with $a=-\infty$.)*

Lemma 4.3. *Let the $n \times n$ symmetric, positive semidefinite matrix $\boldsymbol{B}$ have the eigenvalue 0 with multiplicity k, and let its other eigenvalues be at least ϱ. Let $\boldsymbol{P}$ be an $n \times n$ positive-semidefinite matrix such that $\|\boldsymbol{P}\|=\varepsilon$. Then the $n\times n$ positive-semidefinite matrix $\boldsymbol{C}:=\boldsymbol{B}+\boldsymbol{P}$ has at least k eigenvalues that are at most ε. Furthermore, denoting by $\boldsymbol{y}_1,\ldots,\boldsymbol{y}_k$ the eigenvectors corresponding to the k smallest eigenvalues of $\boldsymbol{C}$ and decomposing them as*

$$\boldsymbol{y}_i=\boldsymbol{u}_i+\boldsymbol{z}_i,\quad \boldsymbol{u}_i\in F,\ \boldsymbol{z}_i\perp F, \tag{4.1}$$

where F is the kernel of $\boldsymbol{B}$, then for the orthogonal components the relation

$$\|\boldsymbol{z}_i\|^2\leqslant\frac{1}{\varrho}\varepsilon\quad (i=1,\ldots,k)$$

holds.

Proof. Let the vector $\boldsymbol{u}\in F$, $\|\boldsymbol{u}\|=1$ be arbitrary. Then, on the one hand,

$$\boldsymbol{u}^{\mathrm{T}}\boldsymbol{Cu}=\boldsymbol{u}^{\mathrm{T}}\boldsymbol{Pu}\leqslant\|\boldsymbol{P}\|\cdot\|\boldsymbol{u}\|^2\leqslant\varepsilon. \tag{4.2}$$

As F is a k-dimensional subspace of R^n, according to Corollary 4.2(b) the matrix $\boldsymbol{C}$ has at least k eigenvalues not greater then ε.

On the other hand, any vector $\boldsymbol{y}\in R^n$ can uniquely be decomposed as $\boldsymbol{y}=\boldsymbol{u}+\boldsymbol{z}$, where $\boldsymbol{u}\in F$ and $\boldsymbol{z}\perp F$. Then

$$\boldsymbol{y}^{\mathrm{T}}\boldsymbol{Cy}=\boldsymbol{y}^{\mathrm{T}}\boldsymbol{By}+\boldsymbol{y}^{\mathrm{T}}\boldsymbol{Py}=\boldsymbol{z}^{\mathrm{T}}\boldsymbol{Bz}+\boldsymbol{y}^{\mathrm{T}}\boldsymbol{Py}\geqslant\varrho\|\boldsymbol{z}\|^2. \tag{4.3}$$

If we choose an orthonormal set $\boldsymbol{y}_1,\ldots,\boldsymbol{y}_k$, the members of which are eigenvectors corresponding to the k smallest eigenvalues (being at most ε) of $\boldsymbol{C}$, then according to formulas (4.2) and (4.3) the inequalities

$$\varepsilon\geqslant\boldsymbol{y}_i^{\mathrm{T}}\boldsymbol{C}\boldsymbol{y}_i\geqslant\varrho\|\boldsymbol{z}_i\|^2\quad(i=1,\ldots,k)$$

hold, which finishes the proof. □

We remark that in the case when there are coincidences among the k smallest eigenvalues of $\boldsymbol{C}$, the statement (4.1) holds for any choice of an orthonormal set of the corresponding eigenvectors.

Lemma 4.4. *Let $F\subset R^n$ be a k-dimensional subspace and $\boldsymbol{y}_1,\ldots,\boldsymbol{y}_k$ be an orthonormal set of vectors in R^n. They are decomposed as*

$$\boldsymbol{y}_i=\boldsymbol{v}_i+\boldsymbol{z}_i,\quad \boldsymbol{v}_i\in F,\ \boldsymbol{z}_i\perp F\quad(i=1,\ldots,k).$$

Then there exists an orthonormal set of vectors $\boldsymbol{u}_1,\ldots,\boldsymbol{u}_k$ within the subspace F such that

$$\sum_{i=1}^{k}\|\boldsymbol{y}_i-\boldsymbol{u}_i\|^2\leqslant 2\sum_{i=1}^{k}\|\boldsymbol{z}_i\|^2.$$

Proof. Let us denote by $\boldsymbol{Y}$ and $\boldsymbol{U}$ the $n\times k$ matrices with column vectors $\boldsymbol{y}_i$'s and $\boldsymbol{u}_i$'s, respectively, where $\{\boldsymbol{u}_1,\ldots,\boldsymbol{u}_n\}$ is an arbitrary orthonormal set of vectors from F. We have to show that there exists a $k\times k$ orthogonal matrix $\boldsymbol{R}$ such that

$$\|\boldsymbol{Y}-\boldsymbol{UR}\|^2\leqslant 2\Delta,$$

where $\Delta:=\sum_{i=1}^{k}\|\boldsymbol{z}_i\|^2$. Denoting the left-hand side by $L(\boldsymbol{R})$, we have

$$\begin{aligned}L(\boldsymbol{R})&=\operatorname{tr}(\boldsymbol{Y}-\boldsymbol{UR})^{\mathrm{T}}(\boldsymbol{Y}-\boldsymbol{UR})\\&=\operatorname{tr}\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y}+\operatorname{tr}\boldsymbol{R}^{\mathrm{T}}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{UR}-2\operatorname{tr}\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{UR}\\&=\operatorname{tr}\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y}+\operatorname{tr}(\boldsymbol{U}^{\mathrm{T}}\boldsymbol{U})(\boldsymbol{RR}^{\mathrm{T}})-2\operatorname{tr}\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{UR}=2(k-\operatorname{tr}\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{UR}).\end{aligned}$$

On the one hand, $L(\boldsymbol{R})$ is minimal, if tr $\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{U}\boldsymbol{R}$ is maximal. The following lemma will be used: let $\boldsymbol{A}$ be a $k\times k$ matrix and $\boldsymbol{R}$ be a $k\times k$ orthogonal one. Then tr$\boldsymbol{A}\boldsymbol{R}$ is maximal, if $\boldsymbol{A}\boldsymbol{R}$ is symmetric and in this case its maximum is equal to the sum of the singular values of the matrix $\boldsymbol{A}$ (for the proof, see [3, p. 67]). This lemma is applied for the matrix $\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{U}$:

$$\min_{\boldsymbol{R}\text{ orthogonal}} L(\boldsymbol{R})=2\sum_{i=1}^{k}(1-s_i),$$

where $0\leqslant s_1\leqslant\dots\leqslant s_k$ are the singular values of the matrix $\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{U}$. On the other hand,

$$\Delta=\|\boldsymbol{Y}-\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{Y}\|^2=\mathrm{tr}(\boldsymbol{Y}-\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{Y})^{\mathrm{T}}(\boldsymbol{Y}-\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{Y})$$

$$=\mathrm{tr}\,\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{Y}-\mathrm{tr}\,\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{U}\boldsymbol{U}^{\mathrm{T}}\boldsymbol{Y}=k-\|\boldsymbol{Y}^{\mathrm{T}}\boldsymbol{U}\|^2=\sum_{i=1}^{k}(1-s_i^2).$$

Now it remains only to show that $1-s_i\leqslant 1-s_i^2$ $(i=1,\dots,k)$. But it holds true, since

$$s_i\leqslant s_k\leqslant s_k(\boldsymbol{Y})\cdot s_k(\boldsymbol{U})=1,$$

the greatest singular values of both $\boldsymbol{Y}$ and $\boldsymbol{U}$ being equal to 1 (moreover, as their columns are orthogonal, they have k singular values which are equal to 1). □

Lemma 4.5. *Let the $n\times n$ symmetric, positive semidefinite matrix $\boldsymbol{B}$ have the eigenvalue λ with multiplicity k, and suppose that its other eigenvalues are outside the interval $(\lambda-\varrho,\lambda+\varrho)$. Let us denote by F the k-dimensional eigenspace corresponding to λ. Let $\boldsymbol{P}$ be $n\times n$ symmetric, positive semidefinite matrix such that $\|\boldsymbol{P}\|=\varepsilon<\varrho$. Then the $n\times n$ symmetric, positive semidefinite matrix $\boldsymbol{C}:=\boldsymbol{B}+\boldsymbol{P}$ has at least k eigenvalues $\kappa_1,\dots,\kappa_k$ in the interval $[\lambda-\varepsilon,\lambda+\varepsilon]$ and for the corresponding eigenvectors $\boldsymbol{y}_1,\dots,\boldsymbol{y}_k$ the relations*

$$d(\boldsymbol{y}_i,F)\leqslant\frac{\varepsilon}{\varrho-\varepsilon}\quad(i=1,\dots,k)$$

hold, where $d(\boldsymbol{y},F)$ denotes the distance of the vector $\boldsymbol{y}$ from the subspace F.

Proof. We shall prove more: on the conditions of the lemma $\boldsymbol{C}$ has exactly k eigenvalues in the interval $[\lambda,\lambda+\varepsilon]$. Let $\boldsymbol{B}$ have p eigenvalues less than and q eigenvalues greater than λ. Then $p+k+q=n$. On the one hand — as $\boldsymbol{P}$ is positive semidefinite — by a perturbation theorem of Rao [10] it follows that the matrix $\boldsymbol{C}=\boldsymbol{B}+\boldsymbol{P}$ has at least $k+q$ eigenvalues greater than λ, at least q ones greater than $\lambda+\varrho$ and p ones less than $\lambda-\varrho+\varepsilon<\lambda$.

On the other hand we shall show that $\boldsymbol{C}$ has at least $p+k$ eigenvalues being at most $\lambda+\varepsilon$. For this purpose let us denote by G the $(p+k)$-dimensional subspace spanned by the eigenvectors $(\boldsymbol{u}_1,\dots,\boldsymbol{u}_{p+k})$ of $\boldsymbol{B}$ corresponding to eigenvalues $\leqslant\lambda$. As any $g\in G$ can be written as $\boldsymbol{g}=\sum_{i=1}^{p+k}\alpha_i\boldsymbol{u}_i$ — where $\sum_{i=1}^{p+k}\alpha_i^2=1$ —,

$$\boldsymbol{g}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{g}=\sum_{i=1}^{p+k}\alpha_i^2\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{B}\boldsymbol{u}_i\leqslant\lambda.$$

Therefore

$$\boldsymbol{g}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{g}=\boldsymbol{g}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{g}+\boldsymbol{g}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{g}\leqslant\lambda+\varepsilon.$$

Applying Corollary 4.2(b) we obtain the required statement.

Comparing the above facts it follows that $\boldsymbol{C}$ has exactly k eigenvalues within $[\lambda,\lambda+\varepsilon]$.

Let $\boldsymbol{u}_1,\dots,\boldsymbol{u}_n$ be pairwise orthonormal eigenvectors of $\boldsymbol{B}$ with eigenvalues $0\leqslant\lambda_1\leqslant\dots\leqslant\lambda_n$, and let $\kappa_1,\dots,\kappa_k$ be eigenvalues of $\boldsymbol{C}$ such that $|\kappa_j-\lambda|\leqslant\varepsilon$, $(j=1,\dots,k)$. Let $\boldsymbol{y}_1,\dots,\boldsymbol{y}_k$ denote the corresponding eigenvectors. Any of them (we denote it simply by $\boldsymbol{y}$ with eigenvalue κ) can uniquely be decomposed as

$$\boldsymbol{y}=\sum_{i=1}^{n}c_i\boldsymbol{u}_i=\sum_{i:\,\lambda_i=\lambda}c_i\boldsymbol{u}_i+\sum_{i:\,\lambda_i\neq\lambda}c_i\boldsymbol{u}_i,$$

where the constants $c_1,\dots,c_n$ are chosen appropriately.

Then, on the one hand,

$$\boldsymbol{C}\boldsymbol{y}=(\boldsymbol{B}+\boldsymbol{P})\boldsymbol{y}=\sum_{i=1}^{n}c_i\lambda_i\boldsymbol{u}_i+\boldsymbol{P}\boldsymbol{y},\tag{4.4}$$

while, on the other hand,

$$\boldsymbol{C}\boldsymbol{y}=\kappa\boldsymbol{y}=\sum_{i=1}^{n}c_i\kappa\boldsymbol{u}_i.\tag{4.5}$$

Comparing equations (4.4) and (4.5) we obtain that

$$\sum_{i=1}^{n}c_i(\kappa-\lambda_i)\boldsymbol{u}_i=\boldsymbol{P}\boldsymbol{y}.$$

Because of the orthogonality of the vectors $\boldsymbol{u}_i$ the Pythagorean theorem can be applied: $\sum_{i=1}^{n}c_i^2(\kappa-\lambda_i)^2=\varepsilon^2$. Since for the indices i's with $\lambda_i=\lambda$ the eigenvectors $\boldsymbol{u}_i$'s are elements of the subspace F and for those with $\lambda_i\neq\lambda$ the vectors $\boldsymbol{u}_i$'s are orthogonal to F, $d^2(\boldsymbol{y},F)=\sum_{i:\,\lambda_i\neq\lambda}c_i^2$. Therefore, in the case of $\varrho>\varepsilon$ the relation

$$(\varrho-\varepsilon)^2d^2(\boldsymbol{y},F)=(\varrho-\varepsilon)^2\sum_{i:\,\lambda_i\neq\lambda}c_i^2\leqslant\sum_{i:\,\lambda_i\neq\lambda}c_i^2(\kappa-\lambda_i)^2\leqslant\sum_{i=1}^{n}c_i^2(\kappa-\lambda_i)^2=\varepsilon^2$$

holds, which implies our statement. □

Corollary 4.6. *Under the assumptions of Lemmas 4.2, 4.3 and 4.5 there exists an orthonormal set $\boldsymbol{u}_1,\dots,\boldsymbol{u}_n\in F$ such that in case* (i),

$$\sum_{i=1}^{k}\|\boldsymbol{y}_i-\boldsymbol{u}_i\|^2\leqslant 2k\frac{\varepsilon}{\varrho},$$

while in case (ii),

$$\sum_{i=1}^{k}\|\boldsymbol{y}_i-\boldsymbol{u}_i\|^2\leqslant 2k\frac{\varepsilon^2}{(\varrho-\varepsilon)^2}$$

holds.

In future we shall denote simply by c the coloring corresponding to the k-partition P_k.

Proof of Theorem 3.4. Let the k-partition P_k be fixed.

(ii) In case (ii) let $F \subset R^n$ be the $(k-1)$-dimensional subspace of the consistent eigenvectors of the λ-ideal matrix $\boldsymbol{B}$. Let $y_1, \dots, y_{k-1}$ denote $k-1$ pairwise orthonormal eigenvectors corresponding to the eigenvalues $\kappa_1, \dots, \kappa_{k-1}$ of the Laplacian $\boldsymbol{C}=\boldsymbol{B}+\boldsymbol{P}$ such that

$$|\kappa_i-\lambda| \leqslant \varepsilon \quad (i=1,\dots,k-1),$$

where $\varepsilon=\|\boldsymbol{P}\|$.

Let us choose one of the vectors y_i's and denote it simply by $y=(y(1),\dots,y(n))^{\mathrm{T}}$, where $y(j)$ stands for its jth coordinate. We are looking for the consistent vector $\boldsymbol{u}\in F$ with respect to the k-partition P_k such that $d^2(y,\boldsymbol{u})=d^2(y,F)$. Since the consistent vector $\boldsymbol{u}$ has n_1 coordinates equal to $t(1)$, n_2 coordinates equal to $t(2),\dots,$ and n_k coordinates equal to $t(k)$, where $\sum_{i=1}^{k} n_i t(i)=0$, the following expression is to be minimized according to $t(1),\dots,t(k)$:

$$\sum_{i=1}^{k} \sum_{j:\, c(j)=i} [y(j)-t(i)]^2.$$

The minimum is attained for the choice

$$t(i)=\frac{\sum_{j:\, c(j)=i} y(j)}{n_i} \quad (i=1,\dots,k).$$

Let us assign in this way to each y_i the consistent vector $\boldsymbol{u}_i$, which realizes its distance from the subspace F. On the one hand we obtain that $\sum_{i=1}^{k-1} d^2(y_i,F)$ is equal to $S_k^2(P_k,X)$, where the $(k-1)$-dimensional representatives of the vertices are determined by the eigenvectors $y_1,\dots,y_{k-1}$: $X=(x_1,\dots,x_n)=(y_1,\dots,y_{k-1})^{\mathrm{T}}$. On the other hand, by means of Lemma 4.5,

$$d^2(y_i,F) \leqslant \frac{\varepsilon^2}{(\varrho-\varepsilon)^2} \quad (i=1,\dots,k-1).$$

By summing it for $i=1,\dots,k-1$, our proof is finished.

(i) In case (i) let $F \subset R^n$ be the k-dimensional subspace being the kernel of the 0-ideal matrix $\boldsymbol{B}$. Let $y_1,\dots,y_k$ denote k pairwise orthonormal eigenvectors corresponding to the k smallest eigenvalues of the Laplacian $\boldsymbol{C}=\boldsymbol{B}+\boldsymbol{P}$. As the eigenvalues of the Laplacian $\boldsymbol{C}$ corresponding to the eigenvectors $y_1,\dots,y_k$ are at most ε, Lemma 4.3 can be applied. With the same argument as in case (ii), we obtain that

$$d^2(y_i,F) \leqslant \frac{\varepsilon}{\varrho} \quad (i=1,\dots,k).$$

By summing it for $i=1,\dots,k$, our proof is complete. □

Proof of Theorem 3.5. (ii) In case (ii) by the notations of the previous proof, and furthermore, by setting $\boldsymbol{U}:=(\boldsymbol{u}_1,\dots,\boldsymbol{u}_{k-1})$ and $\boldsymbol{Y}:=(y_1,\dots,y_{k-1})$ we obtain

$$\chi_k(P_k)=\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{U}, \quad \text{while } \sum_{j=1}^{k-1} \kappa_j=\operatorname{tr} \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{Y}.$$

Therefore, our estimation is as follows:

$$\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{U}-\operatorname{tr} \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{C}\boldsymbol{Y}=[\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{U}-\operatorname{tr} \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{Y}] + [\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{U}-\operatorname{tr} \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{P}\boldsymbol{Y}]. \tag{4.6}$$

The first term in brackets can be estimated from above with

$$\begin{aligned}
\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{U}-\operatorname{tr} \boldsymbol{Y}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{Y} &= \sum_{i=1}^{k-1} \{\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{B}\boldsymbol{u}_i - y_i^{\mathrm{T}}\boldsymbol{B}y_i\} \\
&= \sum_{i=1}^{k-1} \{\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{B}(\boldsymbol{u}_i-y_i)+(\boldsymbol{u}_i-y_i)^{\mathrm{T}}\boldsymbol{B}y_i\} \\
&\leqslant \sum_{i=1}^{k-1} \{\|\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{B}\| \cdot \|\boldsymbol{u}_i-y_i\| + \|\boldsymbol{u}_i-y_i\| \cdot \|\boldsymbol{B}\| \cdot \|y_i\|\} \\
&= (\lambda+\|\boldsymbol{B}\|) \sum_{i=1}^{k-1} \|\boldsymbol{u}_i-y_i\| \leqslant (\lambda+\|\boldsymbol{C}\|) \sum_{i=1}^{k-1} \|\boldsymbol{u}_i-y_i\| \\
&\leqslant (\lambda+\lambda_{n-1})\sqrt{k-1}\sqrt{\sum_{i=1}^{k-1} \|\boldsymbol{u}_i-y_i\|^2} \\
&\leqslant (\lambda+\lambda_{n-1})\sqrt{k-1}\sqrt{2(k-1)\frac{\varepsilon^2}{(\varepsilon-\varrho)^2}},
\end{aligned}$$

where $\lambda_{n-1}=\|\boldsymbol{C}\|$ and we applied Corollary 4.6. The upper estimation of the second term is

$$\begin{aligned}
\sum_{i=1}^{k-1} \{\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{P}\boldsymbol{u}_i - y_i^{\mathrm{T}}\boldsymbol{P}y_i\} &= \sum_{i=1}^{k-1} \{\boldsymbol{u}_i^{\mathrm{T}}\boldsymbol{P}(\boldsymbol{u}_i-y_i)+(\boldsymbol{u}_i-y_i)^{\mathrm{T}}\boldsymbol{P}y_i\} \\
&\leqslant \sum_{i=1}^{k-1} \{\|\boldsymbol{u}_i\| \cdot \|\boldsymbol{P}\| \cdot \|\boldsymbol{u}_i-y_i\| + \|\boldsymbol{u}_i-y_i\| \cdot \|\boldsymbol{P}\| \cdot \|y_i\|\} \\
&= 2\varepsilon \sum_{i=1}^{k-1} \|\boldsymbol{u}_i-y_i\| \leqslant 2\varepsilon\sqrt{k-1}\sqrt{\sum_{i=1}^{k-1} \|\boldsymbol{u}_i-y_i\|^2} \\
&\leqslant 2\varepsilon\sqrt{k-1}\sqrt{2(k-1)\frac{\varepsilon^2}{(\varrho-\varepsilon)^2}}.
\end{aligned} \tag{4.7}$$

After summing the two estimates, the required result is obtained.

(i) In case (i) quite similarly the notations $\boldsymbol{U}:=(\boldsymbol{u}_1,\dots,\boldsymbol{u}_k)$ and $\boldsymbol{Y}:=(y_1,\dots,y_k)$ are introduced. Here the first term of (4.6) in brackets can be estimated from above with 0, as $\operatorname{tr} \boldsymbol{U}^{\mathrm{T}}\boldsymbol{B}\boldsymbol{U}=0$ and $\boldsymbol{B}$ is positive-semidefinite. For the estimation of the second term the counting argument in (4.7) is applied and by the Corollary 4.6 we obtain that it is at most

$$2\varepsilon\sqrt{k}\sqrt{2k\frac{\varepsilon}{\varrho}},$$

which is also the estimation of the whole difference

$$\operatorname{tr} U^{\mathrm{T}}CU-\operatorname{tr} Y^{\mathrm{T}}CY=\tau_k(P_k)-\sum_{j=1}^{k}\lambda_j. \qquad \square$$

Lemma 4.7. *Let $X=(x_1,\ldots,x_n)=(u_1,\ldots,u_{k-1})^{\mathrm{T}}$ be a $(k-1)$-dimensional Euclidean representation of the vertices of the weighted graph $G=(V,W)$ and $P_k=(V_1,\ldots,V_k)$ be any fixed k-partition of the set of vertices. Then the sum of the costs of the monocolored edges with respect to the k-partition P_k is at least $\varrho(P_k)\cdot S_k^2(P_k,X)$, where $\varrho(P_k):=\min_{i=1}^{k}\lambda_1(B_i)$, the matrix B_i being the Laplacian of the weighted subgraph G_i of G induced by V_i (which contains edges of the ith color).*

Proof. The sum of the costs of the edges is decreased if we sum only for the monocolored ones in the partition P_k and this sum is equal to $\operatorname{tr} XBX^{\mathrm{T}}=\sum_{l=1}^{k-1}u_l^{\mathrm{T}}Bu_l$.

Let $u\in R^n$ be an arbitrary vector with $\|u\|=1$ and with $\sum_{j=1}^{n}u(j)=0$, furthermore, let $u^i\in R^{n_i}$ be its ith section with respect to P_k. Then

$$u^{\mathrm{T}}Bu=\sum_{i=1}^{k}u^{i^{\mathrm{T}}}B_iu^i\geqslant\sum_{i=1}^{k}\lambda_1(B_i)\cdot\|u^i\|^2\geqslant\sum_{i=1}^{k}\lambda_1(B_i)\cdot\sigma^2(u^i)$$

$$\geqslant\varrho(P_k)\sum_{i=1}^{k}\sigma^2(u^i)=\varrho(P_k)\cdot S_k^2(P_k,u).$$

In the first inequality we utilized that because of $\sum_{j=1}^{n}u(j)=0$ the quadratic forms $u^{i^{\mathrm{T}}}B_iu^i$ are confined to the ith sections of vectors orthogonal to the vector of 1's. The notations

$$\sigma^2(u^i):=\sum_{j:\,c(j)=i}\left(u(j)-\frac{1}{n_i}\sum_{m:\,c(m)=i}u(m)\right)^2$$

for the variance of the vector u^i and

$$S_k^2(P_k,u):=\sum_{i=1}^{k}\sigma^2(u^i)$$

for the k-variance of the vector u with respect to the k-partition P_k are used. The second inequality follows from the Steiner formula.

Eventually by summing for the vectors $u_1,\ldots,u_{k-1}$ and utilizing that $S_k^2(P_k,X)=\sum_{l=1}^{k-1}S_k^2(P_k,u_l)$, the required result is obtained. $\square$

Proof of Proposition 3.6. Let X^* be an optimal $(k-1)$-dimensional representation of the above weighted graph. Then by the Representation Theorem, the sum of the costs of the edges in this representation is less than $\lambda_1+\cdots+\lambda_{k-1}$, so does the sum of the costs of the monocolored ones. Therefore, Lemma 4.7 can be applied. $\square$

5. The expanding property of the eigenvalues

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

Theorem 5.1. *Let $0=\lambda_0\leqslant\lambda_1<\lambda_2\leqslant\cdots\leqslant\lambda_{n-1}$ denote the eigenvalues of the weighted Laplacian C_D and let u denote the eigenvector corresponding to λ_1. Let $S_2^2(u)$ be the 2-variance of the coordinates of u defined by*

$$S_2^2(u):=\inf_{c,\alpha}\sum_{i=1}^{n}d_i[u_i-c_{\alpha_i}]^2,$$

where u_i denotes the ith coordinate of the vector u, while $c_{\alpha_i}\in R$ and α_i is equal to 1 or to 2. Then $S_2^2(u)\leqslant\lambda_1/\lambda_2$.

Proof. Because of the preliminary assumption for the sum of the weights

$$\sum_{i=1}^{n}d_i=1. \tag{5.1}$$

According to Section 1 for the coordinates of the eigenvector u the conditions

$$\sum_{i=1}^{n}d_iu_i=0 \quad\text{and}\quad \sum_{i=1}^{n}d_iu_i^2=1$$

hold. Now we shall find a vector y with coordinates y_i, $(i=1,\ldots,n)$ such that the conditions

$$\sum_{i=1}^{n}d_iy_i=0 \tag{5.2}$$

and

$$\sum_{i=1}^{n}d_iu_iy_i=0 \tag{5.3}$$

are met. We are looking for y in the form

$$y_i:=|u_i-a|-b \quad (i=1,\ldots,n), \tag{5.4}$$

where a and b are real numbers.

We state that there exist such real numbers a and b for which conditions (5.1) are fulfilled. Our argument is the following: let us suppose that we have found a. Then by means of (5.1) and (5.2) we obtain that

$$b=\sum_{i=1}^{n}d_i|u_i-a|. \tag{5.5}$$

With this choice of b and with the condition (5.3)

$$\sum_{i=1}^{n} d_i u_i |u_i - a| = 0$$

holds. As the left-hand side is a continuous function of a and it is equal to 1, if $a \leqslant \min_i u_i$ and to -1, if $a \geqslant \max_i u_i$, by means of the Bolzano–Weierstrass theorem we obtain that it must have at least one root between $\min_i u_i$ and $\max_i u_i$. Choosing such an a and the corresponding b according to (5.5), the coordinates of the vector y are uniquely determined by (5.4). Put $c_1 := a - b$ and $c_2 = a + b$. It is easy to see that

$$y_i = |u_i - a| - b = \begin{cases} c_1 - u_i, & \text{if } u_i < a \\ u_i - c_2, & \text{if } u_i \geqslant a, \end{cases}$$

therefore

$$|y_i| = \min\{|u_i - c_1|, |u_i - c_2|\} \tag{5.6}$$

holds for all i. Let us define by

$$\sigma^2(y) := \sum_{i=1}^{n} d_i y_i^2$$

the variance of the coordinates of y. As due to (5.6), $\sigma^2(y)$ is one of the terms behind the inf in the expression of $S_2^2(\boldsymbol{u})$, the relation $\sigma^2(y) \geqslant S_2^2(\boldsymbol{u})$ always holds true. Since in the case of $\sigma(y) = 0$ the 2-variance $S_2^2(\boldsymbol{u})$ is also equal to 0, the statement of the theorem is automatically true. Therefore, $\sigma(y) > 0$ can be supposed. Put $z_i := y_i / \sigma(y)$, $(i = 1, \ldots, n)$ and let us denote by $\boldsymbol{z}$ the vector of coordinates z_i's and by $\boldsymbol{x}_i$ the 2-dimensional vector of first coordinate u_i and second coordinate z_i. Furthermore denote $\boldsymbol{X}$ the $2 \times n$ matrix with row vectors $\boldsymbol{u}$ and $\boldsymbol{z}$ respectively and $\boldsymbol{X}^*$ the $2 \times n$ matrix with row vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ respectively, where $\boldsymbol{v}$ is an eigenvector corresponding to λ_2 subject to the usual conditions. Then on the one hand

$$\max_{u_i \neq u_j} \frac{|z_i - z_j|}{|u_i - u_j|} \leqslant \frac{1}{\sigma(y)}, \tag{5.7}$$

since from the definition of y_i it follows that

$$|y_i - y_j| \leqslant |u_i - u_j|, \quad (i \neq j),$$

i.e. $\boldsymbol{y}$ (as function of $\boldsymbol{u}$) fulfils the Lipschitz condition. On the other hand, by the extremal properties of the eigenvalues and by the formulas (1.1) it follows that

$$\frac{\lambda_1 + \lambda_2}{\lambda_1} = \frac{\operatorname{tr} \boldsymbol{X}^* \boldsymbol{C} \boldsymbol{X}^{*\mathrm{T}}}{\boldsymbol{u}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{u}} \leqslant \frac{\operatorname{tr} \boldsymbol{X} \boldsymbol{C} \boldsymbol{X}^{\mathrm{T}}}{\boldsymbol{u}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{u}} = \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} (u_i - u_j)^2}$$

$$= \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} [(u_i - u_j)^2 + (z_i - z_j)^2]}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} (u_i - u_j)^2}$$

$$\leqslant 1 + \max_{u_i \neq u_j} \frac{(z_i - z_j)^2}{(u_i - u_j)^2} \leqslant 1 + \frac{1}{\sigma^2(y)} \leqslant 1 + \frac{1}{S_2^2(\boldsymbol{u})},$$

which finishes the proof. □

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 classification into two clusters of the optimal 1-dimensional representatives of the vertices is.

The theorem also implies that on the condition $\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} = 1$ the relation $S_2^2(\boldsymbol{u}) < 1$ holds, since $\lambda_1 < \lambda_2$ according to our preliminary assumption. In the case of $\lambda_1 = \lambda_2$ there is no use of 1-dimensional Euclidean representation, because the eigenvectors corresponding to this multiple eigenvalue can be chosen within a subspace of at least 2 dimensions. Therefore, the 2-variance in any direction is the same.

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 $\boldsymbol{C}_D$ between the eigenvalues λ_k and λ_{k+1} we would like to prove the following conjecture:

Conjecture 5.2. Let $0 = \lambda_0 \leqslant \lambda_1 \leqslant \cdots \leqslant \lambda_k < \lambda_{k+1} \leqslant \cdots \leqslant \lambda_{n-1}$ be the spectrum of the weighted Laplacian $\boldsymbol{C}_D = \boldsymbol{I}_n - \boldsymbol{D}^{-1/2} \boldsymbol{W} \boldsymbol{D}^{-1/2}$ of the weighted graph G with weight matrix $\boldsymbol{W}$, where $\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} = 1$, $d_i = \sum_{j=1, j \neq i}^{n} w_{ij}$ and $\boldsymbol{D} = \operatorname{diag}(d_1, \ldots, d_n)$. Let $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^* \in R^k$ be optimal k-dimensional representatives of the vertices satisfying the conditions $\sum_{i=1}^{n} d_i \boldsymbol{x}_i^* = 0$ and $\sum_{i=1}^{n} d_i \boldsymbol{x}_i^* \boldsymbol{x}_i^{*\mathrm{T}} = \boldsymbol{I}_k$. Let $S_{k+1}^2(\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*)$ denote the $(k+1)$-variance of the vectors $\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*$. Suppose these vectors form $k+1$ well-separated clusters in the k-dimensional Euclidean space. Then

$$S_{k+1}^2(\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*) \leqslant k \cdot \frac{\lambda_1 + \lambda_2 + \cdots + \lambda_k}{\lambda_{k+1}}, \quad 1 \leqslant k < n-1.$$

For the proof we would need the following

Lemma 5.3. *There exists a transformation $y_i = f(\boldsymbol{x}_i^*)$ such that the function f satisfies the Lipschitz condition, $\sum_{i=1}^{n} d_i y_i = 0$, $\sum_{i=1}^{n} d_i \boldsymbol{x}_i^* y_i = 0$ and $\sigma^2(y) := \sum_{i=1}^{n} d_i y_i^2 \geqslant S_{k+1}^2(\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*)$.*

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 we are not sure whether such construction exists.

If the lemma were true, the proof of Conjecture 5.2 would be the following:

Proof of Conjecture 5.2. $\sigma(y) > 0$ can be supposed, otherwise $S_{k+1}^2(\boldsymbol{x}_1^*, \ldots, \boldsymbol{x}_n^*)$ is also zero, for which the statement of the theorem is true. Let $z_i := y_i / \sigma(y)$, and let the vector $\boldsymbol{x}_i' \in R^{k+1}$ be obtained by adding z_i to the vector $\boldsymbol{x}_i^*$ as last coordinate. Denote by $\boldsymbol{X}'$

the $(k+1)\times n$ matrix of column vectors $x'_1, x'_2, \ldots, x'_n$. Then by the Representation Theorem

$$\begin{aligned}
\lambda_1+\cdots+\lambda_k+\lambda_{k+1} \leqslant \operatorname{tr} X'CX'^{\mathrm{T}} &= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|x'_i-x'_j\|^2 \\
&= \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|x_i^*-x_j^*\|^2 + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}|z_i-z_j|^2 \\
&\leqslant \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|x_i^*-x_j^*\|^2 \\
&\quad + \frac{k}{\sigma(y)}\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|x_i^*-x_j^*\|^2 \\
&= \left(1+\frac{k}{\sigma(y)}\right)(\lambda_1+\cdots+\lambda_k),
\end{aligned}$$

where in the second equality we applied the Pythagorean theorem and the inequality is due to the Lipschitz condition with constant $\sqrt{k}$. From this inequality the required result

$$S_{k+1}^2(x_1^*, \ldots, x_n^*) \leqslant \sigma(y) \leqslant k\cdot\frac{\lambda_1+\cdots+\lambda_k}{\lambda_{k+1}}$$

is immediately obtained. □

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