Research Article

Beyond the Expanders

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Abstract

Expander graphs are widely used in communication problems and construction of error correcting codes. In such graphs, information gets through very quickly. Typically, it is not true for social or biological networks, though we may find a partition of the vertices such that the induced subgraphs on them and the bipartite subgraphs between any pair of them exhibit regular behavior of information flow within or between the vertex subsets. Implications between spectral and regularity properties are discussed.

Keywords: Spectral gap; Spectral clustering; Volume regularity.

1 Introduction

We want to go beyond the expander graphs that – for four decades – have played an important role in communication networks; for a summary, see e.g., Chung [7] and Hoory et al. [10]. Roughly speaking, the expansion property means that each subset of the graph's vertices has "many" neighbors (combinatorial view), and hence, information gets through such a graph very "quickly" (probabilistic view). We will not give exact definitions of an expander here as those contain many parameters which are not used later. We rather refer to the spectral and random walk characterization of such graphs, as discussed, among others by Alon [1], and Meila and Shi [13].

The general framework of an edge-weighted graph will be used. Expanders have a spectral gap bounded away from zero, where – for a connected graph – this gap is defined as the minimum distance between the normalized Laplacian spectrum (apart from the trivial zero eigenvalue) and the endpoints of the [0,2] interval, the possible range of the spectrum. The larger the spectral gap, the more our graph resembles a random graph and exhibits some quasi-random properties, e.g., the edge densities within any subset and between any two subsets of its vertices do not differ too much of what is expected, see the Expander Mixing Lemma 1 of Section 2. Quasi-random properties and spectral gap of random graphs with given expected degrees are discussed in Chung and Graham [8], and Coja-Oghlan and Lanka [9].

However, the spectral gap appears not at the ends of the normalized Laplacian spectrum in case of generalized random or generalized quasi-random graphs that, in the presence of $k \geq 2$ underlying clusters, have k eigenvalues (including the zero) separated from 1, while the bulk of the spectrum is located around 1, see e.g., [5]. These structures are usual in social or biological networks having k clusters of vertices (that belong to social groups or similarly functioning enzymes) such that the edge density within the clusters and between any pair of the clusters is homogeneous. Such a structure is theoretically guaranteed for any large graph by the Szemerédi

Regularity Lemmas [11] with possibly large k, where k does not depend on the number of vertices, it merely depends on the constant ruling the regularity of the cluster pairs.

Our conjecture is that k so-called structural eigenvalues (separated from 1) in the normalized Laplacian spectrum are indications of such a structure, while the near 1 eigenvalues are responsible for the pairwise regularities. The clusters themselves can be recovered by applying the k-means algorithm for the vertex representatives obtained by the eigenvectors corresponding to the structural eigenvalues (apart from the zero). For the $k = 2$ case we will give an exact relation between the eigenvalue separation (of the non-trivial structural eigenvalue from the bulk of the spectrum) and the volume regularity of the cluster pair that is obtained by the k-means algorithm applied for the coordinates of the transformed eigenvector belonging to the non-trivial structural eigenvalue, see Theorem 1 of Section 3. To eliminate the trivial eigenvalue-eigenvector pair, we shall rather use the normalized modularity spectrum of [6] that plays an important role in finding the extrema of some penalized versions of the Newman-Girvan modularity introduced in [14].

2   Preliminaries and statement of purpose

Let $G = (V, \mathbf{W})$ be a graph on n vertices, where the $n \times n$ symmetric matrix $\mathbf{W}$ has nonnegative real entries and zero diagonal. Here w_{ij} is the similarity between vertices i and j, where 0 similarity means no connection/edge at all. A simple graph is a special case of it with 0-1 weights. Without loss of generality

$$\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} = 1 \tag{1}$$

will be supposed. Hence, $\mathbf{W}$ is a joint distribution, with marginal entries

$$d_i = \sum_{j=1}^{n} w_{ij}, \quad i = 1, \ldots, n$$

which are the *generalized vertex degrees* collected in the main diagonal of the diagonal *degree matrix* $\mathbf{D} = \mathtt{diag}\,(\mathbf{d})$, $\mathbf{d} = (d_1, \ldots, d_n)^T$. In [3, 4] we investigated the spectral gap of the *normalized Laplacian* $\mathbf{L}_D = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$, where $\mathbf{I}$ denotes the identity matrix of appropriate size.

Suppose that our graph is connected ($\mathbf{W}$ is irreducible). Let $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n \leq 2$ denote the eigenvalues of the symmetric normalized Laplacian $\mathbf{L}_D$ with corresponding unit-norm, pairwise orthogonal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Namely, $\mathbf{u}_1 = (\sqrt{d_1}, \ldots, \sqrt{d_n})^T = \sqrt{\mathbf{d}}$. In the random walk setup $\mathbf{D}^{-1}\mathbf{W}$ is the transition matrix (its entry in the (i, j)-th position is the conditional probability of moving from vertex i to vertex j in one step, given that we are in i) which is a stochastic matrix with eigenvalues $1 - \lambda_i$ and corresponding eigenvectors $\mathbf{D}^{-1/2}\mathbf{u}_i$ ($i = 1, \ldots, n$). "Good" expanders have a λ_2 bounded away from zero, that also implies the separation of the isoperimetric number

$$h(G) = \min_{U \subset V : \mathtt{Vol}\,(U) \leq \frac{1}{2}} \frac{e(U, \overline{U})}{\mathtt{Vol}\,(U)}, \tag{2}$$

where for $X, Y \subset V$: $e(X, Y) = \sum_{i \in X} \sum_{j \in Y} w_{ij}$ is the weighted cut between X and Y, while $\mathtt{Vol}\,(U) = \sum_{i \in U} d_i$ is the volume of $U \subset V$. In view of (1), $\mathtt{Vol}\,(V) = 1$, this is why the

minimum is taken on vertex sets having volume at most $\frac{1}{2}$. In [4], we proved that

$$\frac{1}{2}\lambda_2 \leq h(G) \leq \min\{1, \sqrt{2\lambda_2}\}, \tag{3}$$

while in the $\lambda_2 \leq 1$ case the stronger upper estimation

$$h(G) \leq \sqrt{\lambda_2(2 - \lambda_2)}$$

holds.

If a network does not have a "large" λ_2 (compared to the natural lower bound), or equivalently – in view of the above inequalities – it has a relatively "small" isoperimetric number, then the 2-partition of the vertices giving the minimum in (2) indicates a bottleneck, or equivalently, a low conductivity edge-set between two disjoint vertex clusters such that the random walk gets through with small probability between them, but – as some equivalent notions will indicate – it is rapidly mixing within the clusters. To find the clusters, the coordinates of the transformed eigenvector $\mathbf{D}^{-1/2}\mathbf{u}_2$ will be used. In [3], we proved that for the weighted 2-variance of this vector's coordinates

$$S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_2) \leq \frac{\lambda_2}{\lambda_3} \tag{4}$$

holds. For a general $2 \leq k \leq n$, the notion of k-variance – in the Analysis of Variance sense – is the following. The weighted k-variance of the k-dimensional vertex representatives $\mathbf{x}_1, \ldots, \mathbf{x}_n$ comprising the row vectors of the $n \times k$ matrix $\mathbf{X}$ is defined as

$$S_k^2(\mathbf{X}) = \min_{P_k \in \mathcal{P}_k} S_k^2(P_k, \mathbf{X}) = \min_{P_k = (V_1, \ldots, V_k)} \sum_{a=1}^{k} \sum_{j \in V_a} d_j \|\mathbf{x}_j - \mathbf{c}_a\|^2,$$

where $\mathbf{c}_a = \frac{1}{\mathtt{Vol}\,(V_a)} \sum_{j \in V_a} d_j \mathbf{x}_j$ is the weighted center of cluster V_a $(a = 1, \ldots, k)$ and $\mathcal{P}_k$ denotes the set of k-partitions of the vertices. We remark that $S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_1, \mathbf{D}^{-1/2}\mathbf{u}_2) = S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_2)$, since $\mathbf{D}^{-1/2}\mathbf{u}_1 = \mathbf{1}$ is the all 1's vector.

The above results were generalized for minimizing the normalized k-way cut

$$f_k(P_k, G) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left(\frac{1}{\mathtt{Vol}\,(V_a)} + \frac{1}{\mathtt{Vol}\,(V_b)}\right) e(V_a, V_b) = k - \sum_{a=1}^{k} \frac{e(V_a, V_a)}{\mathtt{Vol}\,(V_a)} \tag{5}$$

of the k-partition $P_k = (V_1, \ldots, V_k)$ over the set of all possible k-partitions. Hence,

$$f_k(G) = \min_{P_k \in \mathcal{P}_k} f_k(P_k, G)$$

is the *minimum normalized k-way cut* of the underlying weighted graph $G = (V, \mathbf{W})$. In fact, $f_2(G)$ is the symmetric version of the isoperimetric number and $f_2(G) \leq 2h(G)$. In [4] we proved that

$$\sum_{i=1}^{k} \lambda_i \leq f_k(G) \leq c^2 \sum_{i=1}^{k} \lambda_i, \tag{6}$$

where the upper estimation is relevant only in the case when $S_k^2(\mathbf{D}^{-1/2}\mathbf{u}_1, \ldots, \mathbf{D}^{-1/2}\mathbf{u}_k)$ is small enough and the constant c depends on this minimum k-variance of the vertex representatives.

The *normalized Newman-Girvan modularity* is defined in [6] as the penalized version of the Newman-Girvan modularity [14] in the following way. The normalized k-way modularity of $P_k = (V_1, \ldots, V_k)$ is

$$
\begin{aligned}
Q_k(P_k, G) &= \sum_{a=1}^{k} \frac{1}{\mathrm{Vol}\,(V_a)} \sum_{i,j \in V_a} (w_{ij} - d_i d_j) = \sum_{a=1}^{k} \frac{1}{\mathrm{Vol}\,(V_a)} [e(V_a, V_a) - \mathrm{Vol}^2(V_a)] \\
&= \sum_{a=1}^{k} \frac{e(V_a, V_a)}{\mathrm{Vol}\,(V_a)} - 1 = k - 1 - f_k(P_k),
\end{aligned}
\tag{7}
$$

and

$$
Q_k(G) = \max_{P_k \in \mathcal{P}_k} Q_k(P_k, G)
$$

is the *maximum normalized k-way Newman-Girvan modularity* of the underlying weighted graph $G = (V, \mathbf{W})$. For given k, maximizing this modularity is equivalent to minimizing the normalized cut and can be solved by the same spectral technique. In fact, it is more convenient to use the spectral decomposition of the normalized modularity matrix $\mathbf{B}_D = \mathbf{I} - \mathbf{L}_D - \sqrt{\mathbf{d}}\sqrt{\mathbf{d}}^T$ with eigenvalues $\beta_1 \geq \cdots \geq \beta_n$, that are the numbers $1 - \lambda_i$ with eigenvectors $\mathbf{u}_i$ $(i = 2, \ldots, n)$ and the zero with corresponding unit-norm eigenvector $\sqrt{\mathbf{d}}$. In [4, 6], we also show that a spectral gap between λ_k and λ_{k+1} is an indication of k clusters with low inter-cluster connections; further, the intra-cluster connections (w_{ij}) between vertices i and j of the same cluster are higher than expected under the hypothesis of independence (in view of which vertices i and j are connected with probability $d_i d_j$). In the random walk framework, the random walk stays within the clusters with high probability.

Conversely, minimizing the above modularity will result in clusters with high inter- and low intra-cluster connections. In [6], we proved that

$$
\min_{P_k \in \mathcal{P}_k} Q_k(P_k, G) \geq \sum_{i=1}^{k} \beta_{n+1-i}.
\tag{8}
$$

The existence of k "large" (significantly larger than 1) eigenvalues in the normalized Laplacian spectrum, or equivalently, the existence of k negative eigenvalues (separated from 0) in the normalized modularity spectrum is an indication of k clusters with the above property. In the random walk setup: the walk stays within the clusters with low probability.

These two types of network structures are frequently called community or anti-community structure. Some networks exhibit a more general, still regular behavior: the vertices can be classified into k clusters such that the information-flow within them and between any pair of them is homogeneous. In terms of random walks, the walk stays within clusters or switches between clusters with probabilities characteristic for the cluster pair. That is, if the random walk moves from a vertex of cluster V_a to a vertex of cluster V_b, then the probability of doing this does not depend on the actual vertices, it merely depends on their cluster memberships, $a, b = 1, \ldots, k$.

In this context, we examined the following generalized random graph model, that corresponds to the ideal case: given the number of clusters k, the vertices of the graph independently belong to the clusters; further, conditioned on the cluster memberships, vertices $i \in V_a$ and $j \in V_b$ are connected with probability p_{ab}, independently of each other, $1 \leq a, b \leq k$. Applying the results [5] for the spectral characterization of some noisy random graphs, we are able to prove

that the normalized modularity spectrum of a generalized random graph is the following: there exists a positive number $\delta < 1$, independent of n, such that there are exactly $k-1$ so-called structural eigenvalues of $\mathbf{B}_D$ that are greater than $\delta - o(1)$, while all the others are o(1) in absolute value. It is equivalent that $\mathbf{L}_D$ has k eigenvalues (including the zero) separated from 1.

The $k = 1$ case corresponds to quasi-random graphs and the above characterization corresponds to the eigenvalue separation of such graphs, discussed in [8]. The authors also prove some implications between the so-called quasi-random properties. For example, for dense graphs, "good" eigenvalue separation is equivalent to "low" discrepancy (of the induced subgraphs' densities from the overall edge density).

For the $k \geq 2$ case, generalized quasi-random graphs were introduced by Lovász and T. Sós [12]. These graphs are deterministic counterparts of generalized random graphs with the same spectral properties. In fact, the authors define so-called generalized quasi-random graph sequences by means of graph convergence that also implies the convergence of spectra. Though, the spectrum itself does not carry enough information for the cluster structure of the graph, together with some classification properties of the structural eigenvectors it does. We want to prove some implication between the spectral gap and the volume-regularity of the cluster pairs, also using the structural eigenvectors.

The notion of volume regularity was introduced by Alon et al. [2]. We shall use a slightly modified version of this notion.

Definition 1 *Let $G = (V, \mathbf{W})$ be weighted graph with $\text{Vol}(V) = 1$. The disjoint vertex pair (A, B) is α-volume regular if for all $X \subset A$, $Y \subset B$ we have*

$$|e(X, Y) - \rho(A, B)\text{Vol}(X)\text{Vol}(Y)| \leq \alpha\sqrt{\text{Vol}(A)\text{Vol}(B)}, \tag{9}$$

where $\rho(A, B) = \frac{e(A,B)}{\text{Vol}(A)\text{Vol}(B)}$ is the relative inter-cluster density of (A, B).

Our definition was inspired by the Expander Mixing Lemma stated e.g., in [10] for regular graphs and in [7] for simple graphs in the context of quasi-random properties. Now we formulate it for edge-weighted graphs on a general degree sequence. We also include the proof as a preparation for the proof of Theorem 1 of Section 3.

Lemma 1 *(**Expander Mixing Lemma for Weighted Graphs**) Let $G = (V, W)$ be a weighted graph and suppose that $\text{Vol}(V) = 1$. Then for all $X, Y \subset V$:*

$$|e(X, Y) - \text{Vol}(X)\text{Vol}(Y)| \leq \|\mathbf{B}_D\| \cdot \sqrt{\text{Vol}(X)(1 - \text{Vol}(X))\text{Vol}(Y)(1 - \text{Vol}(Y))}$$
$$\leq \|\mathbf{B}_D\| \cdot \sqrt{\text{Vol}(X)\text{Vol}(Y)},$$

where $\|\mathbf{B}_D\|$ is the spectral norm of the normalized modularity matrix of G.

Proof Let $X \subset A$, $Y \subset B$ and $\mathbf{1}_U \in \mathbb{R}^n$ denote the indicator vector of $U \subset V$. Further, $\mathbf{x} := \mathbf{D}^{1/2}\mathbf{1}_X$ and $\mathbf{y} := \mathbf{D}^{1/2}\mathbf{1}_Y$.

We use the spectral decomposition $\mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2} = \sum_{i=1}^n \rho_i \mathbf{u}_i \mathbf{u}_i^T$, where $\rho_i = 1 - \lambda_i$ ($i = 2, \ldots, n$) are eigenvalues of $\mathbf{B}_D$ and $\rho_1 = 1$ with corresponding unit-norm eigenvector $\mathbf{u}_1 = \sqrt{\mathbf{d}} = \mathbf{D}^{1/2}\mathbf{1}$. We remark that $\mathbf{u}_1$ is also an eigenvector of $\mathbf{B}_D$ corresponding to the eigenvalue zero, hence $\|\mathbf{B}_D\| = \max_{i \geq 2}|\rho_i|$. Let $\mathbf{x} = \sum_{i=1}^n a_i \mathbf{u}_i$ and $\mathbf{y} = \sum_{i=1}^n b_i \mathbf{u}_i$ be the expansions of $\mathbf{x}$ and $\mathbf{y}$ in the orthonormal basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$ with coordinates $a_i = \mathbf{x}^T \mathbf{u}_i$ and $b_i = \mathbf{y}^T \mathbf{u}_i$,

respectively. Observe that $a_1 = \texttt{Vol}(X)$, $b_1 = \texttt{Vol}(Y)$ and $\sum_{i=1}^n a_i^2 = \|\mathbf{x}\|^2 = \texttt{Vol}(X)$, $\sum_{i=1}^n b_i^2 = \|\mathbf{y}\|^2 = \texttt{Vol}(Y)$. Based on these,

$$|e(X,Y) - \texttt{Vol}(X)\texttt{Vol}(Y)| = |\sum_{i=2}^n \rho_i a_i b_i| \le \|\mathbf{B}_D\| \cdot |\sum_{i=2}^n a_i b_i|$$

$$\le \|\mathbf{B}_D\| \cdot \sqrt{\sum_{i=2}^n a_i^2 \sum_{i=2}^n b_i^2}$$

$$\le \|\mathbf{B}_D\| \cdot \sqrt{\texttt{Vol}(X)(1 - \texttt{Vol}(X))\texttt{Vol}(Y)(1 - \texttt{Vol}(Y))}$$

$$\le \|\mathbf{B}_D\| \cdot \sqrt{\texttt{Vol}(X)\texttt{Vol}(Y)},$$

where we also used the triangle and the Cauchy-Schwarz inequalities. ∎

We remark that the spectral gap of G is $1 - \|\mathbf{B}_D\|$, hence – in view of Lemma 1 – the density between any two subsets of "good" expanders is near to what is expected. On the contrary, in the above definition of volume regularity, the X, Y pairs are disjoint, and a "small" α indicates that the (A, B) pair is like a bipartite expander, see e.g., [7].

In the next section we shall prove the following statement for the $k = 2$ case: if one eigenvalue jumps out of the bulk of the normalized modularity spectrum, then clustering the coordinates of the corresponding transformed eigenvector into 2 parts (by minimizing the 2-variance of its coordinates) will result in an α-volume regular partition of the vertices, where α depends on the spectral gap.

Our conjecture is that we may go further: if $k - 1$ (so-called structural) eigenvalues jump out of the normalized modularity spectrum, then clustering the representatives of the vertices – obtained by the corresponding eigenvectors in the usual way – into k clusters will result in α-volume regular pairs, where α depends on the spectral gap (between the structural eigenvalues and the bulk of the spectrum) and the k-variance of the vertex representatives based on the eigenvectors corresponding to the structural eigenvalues.

3   Eigenvalue separation and volume regularity (k=2 case)

Theorem 1 *Let $G = (V, \mathbf{W})$ is an edge-weighted graph on n vertices, with generalized degrees $d_1, \dots, d_n$ and $\mathbf{D} = \texttt{diag}(d_1, \dots, d_n)$. Suppose that $\texttt{Vol}(V) = 1$ and there are no dominant vertices: $\max_{1 \le i \le n} d_i = o(1)$ as $n \to \infty$. Let the eigenvalues of $\mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2}$, enumerated in decreasing absolute values, be*

$$1 = \rho_1 > |\rho_2| = \delta > \varepsilon = |\rho_3| \ge |\rho_i|, \quad i \ge 4.$$

The partition (A, B) of V is defined in such a way that it minimizes the weighted 2-variance of the coordinates of $\mathbf{D}^{-1/2}\mathbf{u}$, where $\mathbf{u}$ is the unit-norm eigenvector belonging to ρ_2. Then the (A, B) pair is $\mathcal{O}(\sqrt{\frac{1-\delta}{1-\varepsilon}})$-volume regular.

Remark 1 *The statement of Theorem 1 has relevance only if δ is much larger than ε. In this case the spectral gap between the largest absolute value eigenvalue and the others in the normalized modularity spectrum indicates a regular 2-partition of the graph that can be constructed based on the eigenvector belonging to the structural eigenvalue.*

Remark 2 *The statement of the above theorem also has relevance in the dense case (supported by the condition that there are no dominant vertices). We remark that in the sparse case there is an exceptional set comprising low degree vertices. Authors of [2] prove equivalences of quasi-random properties for the core of the graph (the vertex set deprived of the exceptional set). Using the modularity spectrum of this core, the above theorem remains valid for it.*

Proof of Theorem 1: We use the notations in Lemma 1's proof. Let $X \subset A$, $Y \subset B$. Fort short, $\mathbf{x} := \mathbf{D}^{1/2}\mathbf{1}_X$, $\mathbf{y} := \mathbf{D}^{1/2}\mathbf{1}_Y$, $\mathbf{a} := \mathbf{D}^{1/2}\mathbf{1}_A$, $\mathbf{b} := \mathbf{D}^{1/2}\mathbf{1}_B$. With the notations $\rho = \rho(A, B)$ and $\mathbf{M} = \mathbf{W} - \rho\mathbf{d}\mathbf{d}^T$,

$$|e(X,Y) - \rho\texttt{Vol}\,(X)\texttt{Vol}\,(Y)| = |\mathbf{1}_X^T\mathbf{M}\mathbf{1}_Y| = |\mathbf{x}^T(\mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2} - \rho\sqrt{\mathbf{d}}\sqrt{\mathbf{d}}^T)\mathbf{y}|. \tag{10}$$

Using the spectral decomposition $\mathbf{D}^{-1/2}\mathbf{W}\mathbf{D}^{-1/2} = \sum_{i=1}^{n} \rho_i\mathbf{u}_i\mathbf{u}_i^T$ and the fact that $\mathbf{u}_1 = \sqrt{\mathbf{d}} = \mathbf{D}^{1/2}\mathbf{1}$, we can write (10) as

$$\left|(1-\rho)a_1b_1 + \rho_2 a_2 b_2 + \sum_{i=3}^{n} \rho_i a_i b_i\right|, \tag{11}$$

where $\mathbf{x} = \sum_{i=1}^{n} a_i\mathbf{u}_i$ and $\mathbf{y} = \sum_{i=1}^{n} b_i\mathbf{u}_i$ is the expansion of $\mathbf{x}$ and $\mathbf{y}$ in the orthonormal basis $\mathbf{u}_1, \ldots, \mathbf{u}_n$ with coordinates $a_i = \mathbf{x}^T\mathbf{u}_i$ and $b_i = \mathbf{y}^T\mathbf{u}_i$, respectively.

By Lemma 1, for all $X, Y \subset V$:

$$|\rho(X,Y) - 1| \le \|\mathbf{B}_D\| \cdot \sqrt{\frac{1 - \texttt{Vol}\,(X)}{\texttt{Vol}\,(X)} \cdot \frac{1 - \texttt{Vol}\,(Y)}{\texttt{Vol}\,(Y)}},$$

that is also applicable to the special two-partition $A, B \subset V$ satisfying the postulates. Hence, $|1 - \rho|$ is governed by the spectral norm $|\rho_2|$ of the normalized modularity matrix. In [3], as a by-product of the proof of (4) it came out that to get the partition (A, B), the coordinates of $\mathbf{D}^{-1/2}\mathbf{u}_2$ should be divided into two parts at the median, hence $\texttt{Vol}\,(A)$ and $\texttt{Vol}\,(B)$ are approximately equal to $\frac{1}{2}$ (the approximation is good for large n if the underlying graph does not have dominant vertex-weights). Further, the estimation

$$S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_2) \le \frac{\lambda_2}{\lambda_3} \le \frac{1 - \rho_2}{1 - \varepsilon} \le \frac{1 - \delta}{1 - \varepsilon} \tag{12}$$

also follows. This applies to the $\rho_2 = 1 - \lambda_2$ case. In the $\rho_2 = 1 - \lambda_n$ case, the optimum A, B is obtained by minimizing the 2-variance of the coordinates of the transformed eigenvector $\mathbf{D}^{-1/2}\mathbf{u}_n$ for which the following relation – like (4) – can be proved:

$$S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_n) \le \frac{2 - \lambda_n}{2 - \lambda_{n-1}} \le \frac{\rho_2 + 1}{1 - \varepsilon} \le \frac{1 - \delta}{1 - \varepsilon}, \tag{13}$$

and the optimum cut-point of the coordinates $\mathbf{D}^{-1/2}\mathbf{u}_n$ is also not far from the median. Summarizing, $|1 - \rho| \le |\rho_2| + \eta$, where $\eta = o(1)$.

Therefore, (11) can be estimated from above with

$$|\rho_2| \cdot |a_1 b_1 + a_2 b_2| + \eta a_1 b_1 + \varepsilon \cdot \left|\sum_{i=3}^{n} a_i b_i\right|. \tag{14}$$

As for the second term, $\eta a_1 b_1 = \eta \texttt{Vol}\,(X)\texttt{Vol}\,(Y)$.

Using the Cauchy-Schwarz inequality, the last term can be estimated from above with

$$\varepsilon\sqrt{\sum_{i=3}^{n}a_i^2\sum_{i=3}^{n}b_i^2} \le \varepsilon\sqrt{\sum_{i=2}^{n}a_i^2\sum_{i=2}^{n}b_i^2} \le \varepsilon\sqrt{\texttt{Vol}\,(X)(1-\texttt{Vol}\,(X))\texttt{Vol}\,(Y)(1-\texttt{Vol}\,(Y))}$$

$$\le \varepsilon\sqrt{\texttt{Vol}\,(X)\texttt{Vol}\,(Y)} \le \varepsilon\sqrt{\texttt{Vol}\,(A)\texttt{Vol}\,(B)},$$

since $a_1 = \texttt{Vol}\,(X)$, $b_1 = \texttt{Vol}\,(Y)$ and $\sum_{i=1}^{n}a_i^2 = \|\mathbf{x}\|^2 = \texttt{Vol}\,(X)$, $\sum_{i=1}^{n}b_i^2 = \|\mathbf{y}\|^2 = \texttt{Vol}\,(Y)$.
The first term is reminiscent of an equation for the coordinates of orthogonal vectors. Therefore, we project the vectors $\mathbf{u}_1$, $\mathbf{u}_2$ onto the subspace $F = \texttt{Span}\,\{\mathbf{a}, \mathbf{b}\}$. In fact, $\mathbf{u}_1 = \mathbf{a} + \mathbf{b}$, therefore $\mathbf{u}_1 \in F$. The vector $\mathbf{u}_2$ can be decomposed as

$$\mathbf{u}_2 = \frac{\mathbf{u}_2^T\mathbf{a}}{\texttt{Vol}\,(A)}\mathbf{a} + \frac{\mathbf{u}_2^T\mathbf{b}}{\texttt{Vol}\,(B)}\mathbf{b} + \mathbf{q}, \tag{15}$$

where $\mathbf{q}$ is the component orthogonal to F. For the squared distance $\|\mathbf{q}\|^2$ between $\mathbf{u}_2$ and F, in [3], we proved that it is equal to the weighted 2-variance $S_2^2(\mathbf{D}^{-1/2}\mathbf{u}_2)$ and in (12) we estimated it from above with $\frac{1-\delta}{1-\varepsilon}$. In the $\rho_2 = 1 - \lambda_n$ case similar estimation works using (13). First we estimate $(\mathbf{u}_1^T\mathbf{a})(\mathbf{u}_1^T\mathbf{b}) + (\mathbf{u}_2^T\mathbf{a})(\mathbf{u}_2^T\mathbf{b})$. The problem is that the pairwise orthogonal vectors $\mathbf{u}_1, \mathbf{u}_2$ and $\mathbf{a}, \mathbf{b}$ are not in the same subspace of $\mathbb{R}^n$ as, in general, $\mathbf{u}_2 \notin F$. However, by an argument proved in [3], we can find orthogonal, unit-norm vectors $\tilde{\mathbf{u}}_1, \tilde{\mathbf{u}}_2 \in F$ such that

$$\|\mathbf{u}_1 - \tilde{\mathbf{u}}_1\|^2 + \|\mathbf{u}_2 - \tilde{\mathbf{u}}_2\|^2 \le 2s^2, \tag{16}$$

where, in view of $\mathbf{u}_1 \in F$, $\tilde{\mathbf{u}}_1 = \mathbf{u}_1$. Let $\mathbf{r} := \mathbf{u}_2 - \tilde{\mathbf{u}}_2$. Since $\tilde{\mathbf{u}}_1^T\mathbf{a}, \tilde{\mathbf{u}}_2^T\mathbf{a}$ and $\tilde{\mathbf{u}}_1^T\mathbf{b}, \tilde{\mathbf{u}}_2^T\mathbf{b}$ are coordinates of the orthogonal vectors $\mathbf{a}, \mathbf{b}$ in the basis $\tilde{\mathbf{u}}_1, \tilde{\mathbf{u}}_2$,

$$(\tilde{\mathbf{u}}_1^T\mathbf{a})(\tilde{\mathbf{u}}_1^T\mathbf{b}) + (\tilde{\mathbf{u}}_2^T\mathbf{a})(\tilde{\mathbf{u}}_2^T\mathbf{b}) = 0,$$

and because of $\tilde{\mathbf{u}}_2^T\mathbf{a} + \tilde{\mathbf{u}}_2^T\mathbf{b} = \tilde{\mathbf{u}}_2^T\mathbf{u}_1 = 0$,

$$\tilde{\mathbf{u}}_2^T\mathbf{a} = -\tilde{\mathbf{u}}_2^T\mathbf{b} = \sqrt{\texttt{Vol}\,(A)\texttt{Vol}\,(B)} =: c.$$

Therefore,

$$|(\mathbf{u}_1^T\mathbf{a})(\mathbf{u}_1^T\mathbf{b}) + (\mathbf{u}_2^T\mathbf{a})(\mathbf{u}_2^T\mathbf{b})| = |\texttt{Vol}\,(A)\texttt{Vol}\,(B) + [(\tilde{\mathbf{u}}_2 + \mathbf{r})^T\mathbf{a}][(\tilde{\mathbf{u}}_2 + \mathbf{r})^T\mathbf{b}]|$$

$$= |\texttt{Vol}\,(A)\texttt{Vol}\,(B) + [c + \mathbf{r}^T\mathbf{a}][-c + \mathbf{r}^T\mathbf{b}]| = |c(-\mathbf{r}^T\mathbf{a} + \mathbf{r}^T\mathbf{b}) + (\mathbf{r}^T\mathbf{a})(\mathbf{r}^T\mathbf{b})|$$

$$\le |c|\sqrt{\|\mathbf{r}\|^2\|\mathbf{b} - \mathbf{a}\|^2} + \sqrt{\|\mathbf{r}\|^2\|\mathbf{a}\|^2}\sqrt{\|\mathbf{r}\|^2\|\mathbf{b}\|^2}$$

$$\le \sqrt{\texttt{Vol}\,(A)\texttt{Vol}\,(B)}(|\mathbf{r}\| + \|\mathbf{r}\|^2) \le \sqrt{\texttt{Vol}\,(A)\texttt{Vol}\,(B)}(\sqrt{2}s + 2s^2),$$

using (16) and the fact that $\|\mathbf{b} - \mathbf{a}\|^2 = 1$.

Now we estimate $a_1 b_1 + a_2 b_2 = (\mathbf{u}_1^T\mathbf{x})(\mathbf{u}_1^T\mathbf{y}) + (\mathbf{u}_2^T\mathbf{x})(\mathbf{u}_2^T\mathbf{y})$. Going back to (15) we have

$$\mathbf{u}_2^T\mathbf{x} = \frac{\mathbf{u}_2^T\mathbf{a}}{\texttt{Vol}\,(A)}\mathbf{a}^T\mathbf{x} + \frac{\mathbf{u}_2^T\mathbf{b}}{\texttt{Vol}\,(B)}\mathbf{b}^T\mathbf{x} + \mathbf{q}^T\mathbf{x} = \frac{\texttt{Vol}\,(X)}{\texttt{Vol}\,(A)}\mathbf{u}_2^T\mathbf{a} + \mathbf{q}^T\mathbf{x},$$

and similarly,

$$\mathbf{u}_2^T\mathbf{y} = \frac{\mathbf{u}_2^T\mathbf{a}}{\texttt{Vol}\,(A)}\mathbf{a}^T\mathbf{y} + \frac{\mathbf{u}_2^T\mathbf{b}}{\texttt{Vol}\,(B)}\mathbf{b}^T\mathbf{y} + \mathbf{q}^T\mathbf{y} = \frac{\texttt{Vol}\,(Y)}{\texttt{Vol}\,(B)}\mathbf{u}_2^T\mathbf{b} + \mathbf{q}^T\mathbf{y},$$

that in view of $\|\mathbf{q}\|^2 = s^2$ yields

$$|(\mathbf{u}_1^T\mathbf{x})(\mathbf{u}_1^T\mathbf{y}) + (\mathbf{u}_2^T\mathbf{x})(\mathbf{u}_2^T\mathbf{y})| = |\mathtt{Vol}\,(X)\mathtt{Vol}\,(Y) + (\frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\mathbf{u}_2^T\mathbf{a} + \mathbf{q}^T\mathbf{x})(\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}\mathbf{u}_2^T\mathbf{b} + \mathbf{q}^T\mathbf{y})|$$

$$\leq |\mathtt{Vol}\,(X)\mathtt{Vol}\,(Y) + (\frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\mathbf{u}_2^T\mathbf{a})(\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}\mathbf{u}_2^T\mathbf{b})|$$

$$+ |(\mathbf{q}^T\mathbf{x})(\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}\mathbf{u}_2^T\mathbf{b}) + (\mathbf{q}^T\mathbf{y})(\frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\mathbf{u}_2^T\mathbf{a}) + (\mathbf{q}^T\mathbf{x})(\mathbf{q}^T\mathbf{y})|$$

$$\leq \frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}|\mathtt{Vol}\,(A)\mathtt{Vol}\,(B) + (\mathbf{u}_2^T\mathbf{a})(\mathbf{u}_2^T\mathbf{b})|$$

$$+ \|\mathbf{q}\|\|\mathbf{x}\|\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}\|\mathbf{u}_2\|\|\mathbf{b}\| + \|\mathbf{q}\|\|\mathbf{y}\|\frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\|\mathbf{u}_2\|\|\mathbf{a}\| + \|\mathbf{q}\|^2\|\mathbf{x}\|\|\mathbf{y}\|$$

$$\leq \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}(\sqrt{2}s + 2s^2) + \|\mathbf{q}\|\sqrt{\mathtt{Vol}\,(X)}\frac{\mathtt{Vol}\,(Y)}{\mathtt{Vol}\,(B)}\sqrt{\mathtt{Vol}\,(B)}$$

$$+ \|\mathbf{q}\|\sqrt{\mathtt{Vol}\,(Y)}\frac{\mathtt{Vol}\,(X)}{\mathtt{Vol}\,(A)}\sqrt{\mathtt{Vol}\,(A)} + \|\mathbf{q}\|^2\sqrt{\mathtt{Vol}\,(X)}\sqrt{\mathtt{Vol}\,(Y)}$$

$$= \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}(\sqrt{2}s + 2s^2) + \|\mathbf{q}\|\sqrt{\mathtt{Vol}\,(X)}\sqrt{\mathtt{Vol}\,(Y)}(\frac{\sqrt{\mathtt{Vol}\,(Y)}}{\sqrt{\mathtt{Vol}\,(B)}} + \frac{\sqrt{\mathtt{Vol}\,(X)}}{\sqrt{\mathtt{Vol}\,(A)}} + \|\mathbf{q}\|)$$

$$\leq \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}[(\sqrt{2}s + 2s^2 + s(2 + s)] = \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}[(\sqrt{2} + 2)s + 3s^2]$$

$$\leq \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}(\sqrt{2} + 5)s \leq \sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}(\sqrt{2} + 5)\sqrt{\frac{1 - \delta}{1 - \varepsilon}}.$$

Summarizing, the second and third terms in (14) are estimated from above with $\eta\mathtt{Vol}\,(X)\mathtt{Vol}\,(Y) \leq \eta\sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}$ and $\varepsilon\sqrt{\mathtt{Vol}\,(A)\mathtt{Vol}\,(B)}$, respectively. Because of $\eta = o(1)$ and $\varepsilon < \delta$, by an easy calculation it follows that they are less than $\sqrt{\frac{1-\delta}{1-\varepsilon}}$ for n "large" enough. Therefore, $\alpha = \sqrt{2} + 7$ will do. ∎

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