Matrix and discrepancy view of generalized random and quasirandom graphs

Abstract: We will discuss how graph based matrices are capable to find classification of the graph vertices with small within- and between-cluster discrepancies. The structural eigenvalues together with the corresponding spectral subspaces of the normalized modularity matrix are used to find a block-structure in the graph. The notions are extended to rectangular arrays of nonnegative entries and to directed graphs. We also investigate relations between spectral properties, multiway discrepancies, and degree distribution of generalized random graphs. These properties are regarded as generalized quasirandom properties, and we conjecture and partly prove that they are also equivalent for certain deterministic graph sequences, irrespective of stochastic models.

Keywords: modularity matrix, spectral clustering, multiway discrepancy, generalized random graphs, generalized quasirandom properties

1 Introduction

One may think of random graphs as very disordered. However, we will show, that generalized random graphs have almost sure properties which are related to their spectra, discrepancies, vertex-degrees, and exhibit regular patterns at the expectation. The generalized random graph model, sometimes called stochastic block-model, was first introduced in [24], and discussed later in [4, 15, 22, 27, 30, 33]. This model is the generalization of the classical Erdős–Rényi random graph, the first random graph of the history introduced in [23] and also discussed in [13], which corresponds to the one-cluster case.

The graph $G_n(\mathcal{P}, \mathcal{P}_k)$ on $n$ vertices is a generalized random graph with $k \times k$ symmetric probability matrix $\mathcal{P} = (p_{uv})$ and proper $k$-partition $\mathcal{P}_k = (C_1, \ldots, C_k)$ of the vertices ($|C_u| = n_u$) if vertices of $C_u$ and $C_v$ are connected independently, with probability $p_{uv}$, $1 \leq u < v \leq k$; further, any pair of the vertices within $C_u$ is connected with probability $p_{uu}$ ($u = 1, \ldots, k$). Therefore, the subgraph of $G_n(\mathcal{P}, \mathcal{P}_k)$ confined to the vertex set $C_u$ is an Erdős–Rényi type random graph $G_{n_u}(p_{uu})$, while the bipartite subgraphs connecting vertices of $C_u$ and $C_v$ ($u \neq v$) are random bipartite graphs of edge probability $p_{uv}$. Sometimes we refer to $\mathcal{P}_k$ as clustering, where $C_1, \ldots, C_k$ are the clusters.

In Chapter 3 of [8] we proved that for a given positive integer $k \leq n$, there are almost surely $k$ outstanding, so-called structural eigenvalues in the adjacency, and $k - 1$ outstanding ones in the normalized modularity spectrum of the generalized random graph $G_n(\mathcal{P}, \mathcal{P}_k)$ as $n \to \infty$ under some balancing conditions on the cluster sizes. Under the same conditions, the $k$-variances of the vertex representatives, constructed by the eigen-subspaces corresponding to the structural eigenvalues, is $o(1)$. The $k$-way discrepancy of $G_n(\mathcal{P}, \mathcal{P}_k)$ also tends to 0, and the subgraphs and bipartite subgraphs defined...
on the vertex classes are asymptotically regular and biregular, respectively. These properties can be regarded as so-called generalized quasirandom properties, provided their equivalence can be proved for any graph sequence. More precisely, we focus on an expanding family of graphs such that, for them, any of the above properties implies the others, regardless of stochastic models. In the $k = 1$ case these are called quasirandom or pseudorandom graph sequences and were first discussed by Thomason [36], later, by Chung, Graham and Wilson [19, 20], also by Lovász [29]. In the $k > 1$ case, the deterministic counterparts of the generalized random graphs were first defined in [28] as graph sequences converging to a vertex- and edge-weighted graph (vertex-weights correspond to the relative sizes of the partition-members, whereas edge-weights to the probability matrix) in the sense of the homomorphism densities. Due to convergence facts on spectra [17], the generalized quasirandom graphs are spectrally equivalent to the generalized random graphs.

In the spirit of the Szemerédi regularity lemma [35], given a large graph, we look for a $k$-partition of its vertices, such that the induced subgraphs and bipartite subgraphs be nearly quasirandom, in terms of the discrepancy. For this purpose, we define the $k$-way discrepancy that can be related to spectra. Based on the multiway discrepancy and spectra together with spectral subspaces, we will formulate quasirandom properties and conjecture their equivalences, irrespective of stochastic models. Real-life expanding graph sequences asymptotically capturing one of these properties are random-like, confined to the subgraphs and bipartite subgraphs of them. The equivalences also suggest that spectral methods are capable to find $k$-partitions of the vertices with small within- and between-cluster discrepancies; further, help us to find the optimal $k$ based on gaps within the spectrum. The novel idea is that large, real-life graphs are instances of expanding graph sequences, and if there is a cluster structure behind them, then we are able to recover it by spectral techniques.

The scope of the paper is twofold: partly we want to establish the equivalence of generalized quasirandom properties based on former results of others [19, 20] and Chapter 3 of [8], and partly to make up for the missing chains in the implications. In Proposition 2, we also give a short proof for the Expander Mixing Lemma for irregular graphs, and in Theorem 1, we estimate the $k$-th largest singular value of the normalized matrix with the $k$-way discrepancy. We will also extend the notion of multiway discrepancy to rectangular arrays, of which undirected or directed, unweighted or weighted graphs are special cases. The results are supported by computer simulations and processing migration data on the directed graph of which the spectral relaxation technique is illustrated.

The organization of the paper is as follows. In Section 2, we introduce the notion of graph-based matrices, together with their spectra, spectral subspaces, and corresponding spectral clustering techniques. In Section 3, we discuss the generalized random and quasirandom graphs, together with properties related to spectra, discrepancies and vertex degrees. In Conjecture 1 we state the equivalence of these properties, which are partly known, partly proved in this paper; in fact, only the relation to the vertex-degrees is missing. Particularly, in Section 4, we prove a relation between the $k$-th largest singular value of the normalized matrix and the $k$-way discrepancy of this matrix, which is the key to prove an important implication between the quasirandom properties. In Section 5, we summarize the ideas of the paper.

## 2 Notation and graph based matrices

The notion of the modularity matrix was first introduced for simple graphs (see Newman [31] for an overview) to capture the so-called community structure in social networks. In [7] we extended this notion to weighted graphs as follows. Let $G = (V, W)$ be an edge-weighted graph on the $n$-element vertex-set $V$ with the $n \times n$ symmetric weight-matrix $W$; the entries satisfy $w_{ij} = w_{ji} \geq 0$, $w_{ii} = 0$ and they are similarities between the vertex-pairs. The modularity matrix of $G$ is defined as $M = W - dd^T$, where the entries of $d$ are the generalized vertex-degrees $d_i = \sum_{j=1}^n w_{ij}$ ($i = 1, \ldots, n$). Here $W$ is normalized in such a way that $\sum_{i=1}^n \sum_{j=1}^n w_{ij} = 1$, an assumption that does not hurt the generality, since the following
normalized modularity matrix, to be mostly used, is not affected by the scaling of the entries of $W$:

$$M_D = D^{-1/2}MD^{-1/2},$$

where $D = \text{diag}(d_1, \ldots, d_n)$ is the diagonal degree-matrix. We will demonstrate that the modularity matrix is capable to measure the discrepancy of the underlying graph, a notion which becomes important if we want to find homogeneous patterns in the graph. First we introduce some further notions.

An edge-weighted graph is called connected if its vertices cannot be divided into two disjoint subsets with all zero weights between them. This is equivalent to the weight matrix $W$ being irreducible, in which case, the generalized vertex-degrees are all positive. The modularity matrix $M$ always has a zero eigenvalue with eigenvector $1_n = (1, \ldots, 1)^T$, since its rows sum to zero. Because of $\text{tr}(M) < 0$, $M$ must have at least one negative eigenvalue, and it is usually indefinite. In [11] we proved that the modularity matrix of a simple graph is negative semidefinite if and only if it is a complete multipartite graph. The same applies to the normalized modularity matrix, since it has the same inertia. In [8] we proved that the eigenvalues of $M_D$ are in the $[-1, 1]$ interval, and 1 cannot be an eigenvalue if $G$ is connected. $M_D$ is closely related to the normalized Laplacian matrix. The normalized Laplacian of $G = (V, W)$ is defined as $L_D = I - D^{-1/2}WD^{-1/2}$, and the following relation can be established between the spectra of $L_D$ and $M_D$ when $G$ is connected. Let $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$ denote the eigenvalues of $L_D$. The zero is a single eigenvalue with corresponding unit-norm eigenvector $\sqrt{d} := (\sqrt{d_1}, \ldots, \sqrt{d_n})^T$. The 15 eigenvalues of $M_D$ are the numbers $1 - \lambda_i$ with the same eigenvectors $(i = 1, \ldots, n - 1)$; further, the zero with corresponding unit-norm eigenvector $\sqrt{d}$.

Let $1 < k < n$ be a fixed integer. Usual spectral clustering techniques use the $k$ bottom eigenvalues $\lambda_0, \ldots, \lambda_{k-1}$ of $L_D$ together with the corresponding eigenvectors to find $k$ ‘loosely connected’ clusters of the vertices; about this so-called spectral relaxation of the minimum $k$-way normalized cut problem see, e.g., Chapter 2 of [8]. More generally, in the modularity based spectral clustering, we look for the proper $k$-partition $C_1, \ldots, C_k$ of the vertices such that the within- and between cluster discrepancies are minimized.

To motivate the introduction of the exact discrepancy measure observe that the $ij$ entry of $M$ is $w_{ij} - d_id_j$, which is the difference between the actual connection of the vertices $i, j$ and the connection that is expected under independent attachment of them with probabilities $d_i$ and $d_j$, respectively. Consequently, the difference between the actual and the expected connectedness of the subsets $X, Y \subset V$ is

$$\sum_{i \in X} \sum_{j \in Y} (w_{ij} - d_id_j) = w(X, Y) - \text{Vol}(X)\text{Vol}(Y),$$

where $w(X, Y) = \sum_{i \in X} \sum_{j \in Y} w_{ij}$ is the weighted cut between $X$ and $Y$, and $\text{Vol}(X) = \sum_{i \in X} d_i$ is the volume of the vertex-subset $X$. Further, let $\rho(X, Y) := \frac{w(X, Y)}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}}$ be the density between $X$ and $Y$.

**Definition 1.** The multiway discrepancy of the edge-weighted graph $G = (V, W)$ in the clustering $C_1, \ldots, C_k$ of its vertices is

$$\text{disc}(G; C_1, \ldots, C_k) = \max_{1 \leq u \leq v \leq k} \max_{X \subset C_u, Y \subset C_v} \text{disc}(X, Y; C_u, C_v),$$

$$\text{disc}(X, Y; C_u, C_v) = \frac{|w(X, Y) - \rho(C_u, C_v)\text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}}$$

$$= |\rho(X, Y) - \rho(C_u, C_v)|\sqrt{\text{Vol}(X)\text{Vol}(Y)}. \quad (2)$$

The minimum $k$-way discrepancy of $G$ is

$$\text{disc}_k(G) = \min_{(C_1, \ldots, C_k)} \text{disc}(G; C_1, \ldots, C_k).$$

Note that $\text{disc}(G; C_1, \ldots, C_k)$ is the smallest $\alpha$ such that for every $C_u, C_v$ pair and for every $X \subset C_u, Y \subset C_v$,

$$|w(X, Y) - \rho(C_u, C_v)\text{Vol}(X)\text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(X)\text{Vol}(Y)} \quad (3)$$
holds. Hence, in the \( k \)-partition of the vertices, giving the minimum \( k \)-way discrepancy of \( G \), every \( C_u, C_v \) pair is so-called \( \alpha \)-volume regular (see [2]), and this is the smallest possible discrepancy that can be attained with proper \( k \)-partitions of the vertices of \( G \). It resembles the notion of \( \epsilon \)-regular pairs in the Szemerédi regularity lemma [35], albeit with given number of vertex-clusters, which are usually not equitable; further, with volumes, instead of cardinalities.

In Section 4, we will justify for the following spectral approximation of the minimum \( k \)-way discrepancy problem. Let the eigenvalues of \( \mathbf{M}_D \), enumerated in decreasing absolute values, be \( 1 > |\mu_1| \geq |\mu_2| \geq \cdots \geq |\mu_n| = 0 \). Assume that \( |\mu_{k-1}| > |\mu_k| \), and denote by \( \mathbf{u}_1, \ldots, \mathbf{u}_{k-1} \) the corresponding unit-norm, pairwise orthogonal eigenvectors. Let \( \mathbf{r}_1, \ldots, \mathbf{r}_n \in \mathbb{R}^{k-1} \) be the row vectors of the \( n \times (k - 1) \) matrix of column vectors \( \mathbf{D}^{-1/2} \mathbf{u}_1, \ldots, \mathbf{D}^{-1/2} \mathbf{u}_{k-1} \); they are called \((k - 1)\)-dimensional representatives of the vertices.

The weighted \( k \)-variance of these representatives is defined as

\[
\tilde{S}_k^2 = \min_{(C_1, \ldots, C_k)} \sum_{u=1}^{k} \sum_{j \in C_u} d_j \| \mathbf{r}_j - \mathbf{c}_u \|^2,
\]

where \( \mathbf{c}_u = \frac{1}{\text{vol}(C_u)} \sum_{j \in C_u} d_j \mathbf{r}_j \) is the weighted center of the cluster \( C_u \). It is the weighted \( k \)-means algorithm that gives this minimum, and the point is that the optimum \( \tilde{S}_k \) is just the minimum distance between the eigensubspace corresponding to \( \mu_0, \ldots, \mu_{k-1} \) and the one of the suitably transformed step-vectors over the \( k \)-partitions of \( V \). In Chapter 2 of [8] we also discussed that, in view of subspace perturbation theorems, the larger the gap between \( |\mu_{k-1}| \) and \( |\mu_k| \), the smaller \( \tilde{S}_k \) is. In the \( k \)-partition, which gives the minimum weighted \( k \)-variance of \( G \), the \( k \)-way discrepancy of \( G \) is also ‘fairly small’. The exact relations are established in Section 4, and the message is, that here the eigenvectors corresponding to the largest absolute value eigenvalues have to be used, unlike usual spectral clustering techniques.

In Section 3, we will also need the plain \( k \)-variance of the representatives \( \mathbf{r}_1, \ldots, \mathbf{r}_n \in \mathbb{R}^k \) that are row-vectors of the matrix, the columns of which are the unit-norm, pairwise orthogonal eigenvectors corresponding to the \( k \) largest absolute value eigenvalues of \( \mathbf{W} \). This \( k \)-variance is

\[
S_k^2 = \min_{(C_1, \ldots, C_k)} \sum_{u=1}^{k} \sum_{j \in C_u} \| \mathbf{r}_j - \mathbf{c}_u \|^2,
\]

where \( \mathbf{c}_u = \frac{1}{|C_u|} \sum_{j \in C_u} \mathbf{r}_j \) is the center of the cluster \( C_u \). It is the usual \( k \)-means algorithm that finds this minimum. In fact, under some conditions, there are variants of this algorithm which find a clustering ‘close’ to the optimal one in polynomial time. We will not discuss these algorithmic aspects, see, e.g., [26] for details.

## 3 Generalized random and quasirandom graphs

Generalized random and quasirandom graphs are specimens, where the ‘large’ spectral gap an and the ‘small’ \( k \)-variance show up together with ‘small’ \( k \)-way discrepancy.

**Definition 2.** Let \( n \) be a natural number and \( k \leq n \) be a positive integer. The graph \( G_n(\mathbf{P}, \mathcal{P}_k) \) is a generalized random graph with probability matrix \( \mathbf{P} \) and proper \( k \)-partition \( \mathcal{P}_k = (C_1, \ldots, C_k) \) of the vertices if it satisfies the following. The vertex set is \( V \), \( |V| = n \); the \( k \times k \) symmetric matrix \( \mathbf{P} \) is such that its entries satisfy \( 0 \leq p_{uv} \leq 1 \) (\( 1 \leq u \leq v \leq k \)). Then vertices of \( C_u \) and \( C_v \) are connected independently, with probability \( p_{uv} \), \( 1 \leq u < v \leq k \); further, any pair of the vertices of \( C_u \) is connected with probability \( p_{uu} \) (\( u = 1, \ldots, k \)).

With different notation, this definition can be found, e.g., in [4, 22, 27, 30, 33]. Sometimes it is called stochastic block-model that was first mentioned in [24], and discussed much later in [15] as a special
case of an inhomogeneous random graph. Note that this model is the generalization of the classical Erdős–Rényi random graph, the first random graph of the history introduced in [23] and also discussed in [13], which corresponds to the $k = 1$ case. In this case, the probability matrix boils down to the number $0 < p < 1$, whereas edges come into existence independently, with the same probability $p$; it is denoted by $G_n(p)$.

Note that that Definition 2 makes sense if the probability matrix $P$ contains at least one non-zero entry. In many cases, one or more entries of $P$ are zeros. In particular, when $p_{uu} = 0$ ($u = 1, \ldots, k$) and $p_{uv} = p \in (0, 1)$, then the graph $G_n(P, P_k)$ has a so-called soft-core multipartite structure, defined in [11]. In the special case when $p = 1$, it is the complete $k$-partite graph $K_{n_1, \ldots, n_k}$ over the independent vertex classes of $P_k$, where $n_i = |C_i|$ ($i = 1, \ldots, k$).

If $k = n$ and $p_{ij} := d_id_j / \sum_{m=1}^n d_m$ ($i, j = 1, \ldots, n$), then the model gives the random graph with expected degree sequence $d_1, \ldots, d_n$, first discussed in [21] on the condition that $\max_i d_i^2 \leq \sum_{i=1}^n d_i$. This is a good model for capturing power law graphs in that the random power law graph, introduced in [8], is a special case of it.

However, the generalized random graph model can better be exploited in applications where $k$ is much less than $n$. Now, we keep $k$ and $P$ fixed, while $n \to \infty$ under some balancing conditions on the cluster sizes. In [5, 6, 8] we proved the following properties of a generalized random graph.

**Proposition 1.** Let $G_n(P, P_k)$ be a generalized random graph on $n$ vertices with vertex-classes $P_k = (C_1, \ldots, C_k)$ of sizes $n_1, \ldots, n_k$ and $k \times k$ symmetric probability matrix $P$. Let $k$ be a fixed positive integer and $n \to \infty$ in such a way that $\frac{n_i}{n} \geq c$ ($u = 1, \ldots, k$) with some constant $0 < c \leq \frac{1}{k}$ (called balancing condition). Then the following hold almost surely for the adjacency matrix $A_n$ and the normalized modularity matrix $M_{D,n}$ of $G_n(P, P_k)$.

1. $A_n$ has $k$ so-called structural eigenvalues that are $\Theta(n)$, while the remaining eigenvalues are $O(\sqrt{n})$ in absolute value. Further, the $k$-variance $S_{k,n}^2$ of the $k$-dimensional vertex representatives, based on the eigenvectors corresponding to the structural eigenvalues of $A_n$ (see (5)), is $O(\frac{1}{k})$.

2. There exists a positive constant $0 < \delta < 1$ independent of $n$ (it only depends on $k$) such that $M_{D,n}$ has exactly $k - 1$ structural eigenvalues of absolute value greater than $\delta$, while all the other eigenvalues are less than $n^{-\tau}$ in absolute value, for every $0 < \tau < \frac{1}{2}$. Further, the weighted $k$-variance $S_{k,n}^2$ of the $(k-1)$-dimensional vertex representatives, based on the transformed eigenvectors corresponding to the structural eigenvalues of $M_{D,n}$ (see (4)), is $O(n^{-\tau})$.

3. There is a constant $0 < \theta < 1$ (independent of $n$) such that $\text{disc}_1(G_n(P, P_k)) > \theta, \ldots, \text{disc}_{k-1}(G_n(P, P_k)) > \theta$, and the $k$-way discrepancy $\text{disc}_k(G_n(P, P_k); C_1, \ldots, C_k)$ is $O(n^{-\tau})$.

4. For every $1 \leq u \leq v \leq k$ and $i \in C_u$:

$$\sum_{j \in C_v} a_{ij} = p_{uv}n_v + o(n).$$

For every $1 \leq u \leq v \leq k$ and $i, j \in C_u$:

$$\sum_{\ell \in C_v} a_{ij}a_{\ell j} = p_{uv}^2n_v + o(n).$$

For the proofs of Properties 1-2 see Theorems 3.1.6, 3.1.8 and Propositions 3.1.10, 3.1.12 of [8]. The 2-3 relation between discrepancy and spectra will be discussed in Section 4, whereas the proof of Property 4 is as follows. We will use the following version of the Chernoff’s inequality.

**Lemma 1** (Chernoff inequality for large deviations). Let $X_1, \ldots, X_n$ be independent random variables, $|X_i| \leq K$, $X := \sum_{i=1}^n X_i$. Then for every $a > 0$:

$$P \left( \left| X - \mathbb{E}(X) \right| > a \right) \leq e^{-\frac{a^2}{K^2 + 3Ka/\sqrt{n}}}. $$

**Proof of Property 4.** Consider the generalized random graph sequence $G_n(P, P_k)$, the subgraphs and the bipartite subgraphs of which have the following expected degrees. We will drop the index $n$, and use
the notation $A = (a_{ij})$ for the entries of its adjacency matrix. As for the $C_u, C_v$ pair ($1 \leq u \leq v \leq k$), for any $i \in C_u$, the average degree of $i$ with regard to $C_v$ is

$$\mathbb{E}(\sum_{j \in C_v} a_{ij}) = n_v p_{uv},$$

each vertex in $C_u$ has the same expected number of neighbors in $C_v$.

Observe that for $i \in C_u$, the sum $\sum_{j \in C_v} a_{ij}$ has binomial distribution with the above expectation and variance $n_v p_{uv}(1 - p_{uv})$. Therefore, by Lemma 1, the between-cluster average degrees are highly concentrated on their expectations as $n \to \infty$ under the balancing conditions $\frac{n}{n} \geq c (u = 1, \ldots, k)$ for the cluster sizes. Indeed, for any $0 < \varepsilon < 1$:

$$\mathbb{P}(\left| \frac{1}{n_v} \sum_{j \in C_v} a_{ij} - p_{uv} \right| > \varepsilon) = \mathbb{P}(\left| \sum_{j \in C_v} a_{ij} - n_v p_{uv} \right| > n_v \varepsilon) \leq e^{-\frac{2 n_v (1 - p_{uv}) \varepsilon^2}{e n_v p_{uv}(1 - p_{uv})}}$$

that tends to 0 even with the choice $\varepsilon = n^{-\tau}$, $0 < \tau < \frac{1}{2}$. Therefore, it holds almost surely that

$$\left| \sum_{j \in C_v} a_{ij} - n_v p_{uv} \right| \leq n_v n^{-\tau} = \frac{n}{n} n^{1-\tau} = o(n).$$

This finishes the proof.

As for every $1 \leq u \leq v \leq k$, the number of common neighbors in $C_v$ of any $i, j \in C_u$ ($i \neq j$) pair has binomial distribution with expectation $n_v p_{uv}^2$ and variance $n_v p_{uv}^2(1 - p_{uv}^2)$, with the same calculations as above we obtain that

$$\left| \sum_{t \in C_v} a_{it} a_{jt} - p_{uv}^2 n_v \right| = o(n)$$

almost surely. This finishes the proof.

Consequently, the subgraphs confined to the vertex-classes exhibit regular, while the induced bipartite subgraphs of a generalized random graph exhibit biregular structure asymptotically.

Now we will discuss similar properties of the generalized quasirandom graphs, which are the deterministic counterparts of the generalized random graphs and are spectrally equivalent to them.

Let us start with the $k = 1$ case. Quasirandom or pseudorandom graph sequences were first discussed by Thomason [36]. Later, Chung, Graham and Wilson [19] used the term quasirandom for simple graphs that satisfy any of some equivalent properties, where these properties are closely related to the properties of expander graphs, including the ‘large’ spectral gap. For a sampler of these quasirandom properties see also Lovász [29]. Chung and Graham [20] investigated quasirandom graphs with given degree sequences. Among others, they proved that small discrepancy is caused by a large spectral gap, which is $1 - \|M_D\|$. This relation is summarized in the following proposition that is a straightforward generalization of the Expander Mixing Lemma for irregular graphs.

**Proposition 2.**

$$\text{disc}(G) = \text{disc}_1(G) \leq \|M_D\| = |\mu_1|,$$

where $\|M_D\|$ is the spectral norm of the normalized modularity matrix of $G$.

Though, with different notation, even a stronger version of this proposition is proved in [20], we give another short proof here.

**Proof.** Via separation theorems for singular values, the largest singular value $|\mu_1|$ of $M_D$ is the maximum of the bilinear form $v^T M_D u$ over the unit sphere. Let $X, Y \subset V$ be arbitrary, and denote by $1_X, 1_Y \in \mathbb{R}^n$ the indicator vectors of them. Then

$$\|M_D\| = \max_{\|u\| = \|v\| = 1} |v^T M_D u| \geq \left\| \frac{D^{1/2} 1_X}{\|D^{1/2} 1_X\|} \right\|^T M_D \left( \frac{D^{1/2} 1_Y}{\|D^{1/2} 1_Y\|} \right) = \frac{\|1^T_X M 1_Y\|}{\|D^{1/2} 1_X\| \cdot \|D^{1/2} 1_Y\|} = \frac{|w(X, Y) - \text{Vol}(X) \text{Vol}(Y)|}{\sqrt{\text{Vol}(X) \sqrt{\text{Vol}(Y)}}}. $$
Taking the maxima on the right-hand side over subsets $X, Y \subset V$, the desired relation follows. Note that the estimate is also valid if we take maxima over disjoint $X, Y$ pairs only.

In [20], the authors also proved that in the case of dense enough graphs (the minimum degree is $cn$ for some constant $c$ and number of vertices $n$) the converse implication is also true. In view of the Expander Mixing Lemma, a 'large' spectral gap is an indication that the weighted cut between any two subsets of the graph is near to what is expected in a random graph, the vertices of which are connected independently, with probability proportional to their generalized degrees. The notion of discrepancy together with the Expander Mixing Lemma was first used for simple (sometimes regular) graphs, see e.g., [1, 25], and extended to Hermitian matrices in [14]. Historically, Thomason [36, 37] was the first to prove equivalences between quasirandom properties, though, with a bit different notions: he used the term jumbled graph and not discrepancy.

The multiclass extension of quasirandomness ($k > 1$) is discussed thoroughly in Lovász and Sós [28], where the generalized quasirandom graphs are defined. Here the clusters or cluster-pairs of small discrepancy behave like expanders or bipartite expanders. In fact, these are the deterministic counterparts of quasirandomness and the partitions of the seminal Szemerédi regularity lemma [35]. For the definition, the notion of the convergence of edge- and vertex-weighted graph sequences is needed. Without going into details, we will use the notion of graph convergence as discussed in [16].

The sequence $(G_n)$ of edge- and possibly vertex-weighted graphs is said to be convergent if the sequence $t(F, G_n)$ of homomorphism densities converges for any simple graph $F$ as $n \to \infty$. They also define the limit object that is a symmetric, bounded, measurable function $W : [0, 1] \times [0, 1] \to \mathbb{R}$, called graphon. The stepfunction graphon $W_G$ is assigned to the weighted graph $G$ in the following way: the sides of the unit square are divided into intervals $I_1, \ldots, I_n$ of lengths of the relative vertex-weights, and over the rectangle $I_i \times I_j$ the stepfunction takes on the value that is the edge-weight between vertices $i$ and $j$. The convergence of $(G_n)$ is also equivalent that the stepfunction graphon $W_G$ converges to the limiting graphon in the so-called cut-metric. Roughly speaking, the members of a convergent graph sequence become more and more similar in small details. In terms of the graph convergence, in Section 4 of [8] we proved the following.

**Proposition 3.** Consider the generalized random graph sequence $G_n(P, P_k)$ with $P_k = (C_1, \ldots, C_k)$, $|C_u| = n_u (u = 1, \ldots, k)$. Let $n \to \infty$ in such a way that $\frac{n_u}{n} \to r_u$ with some $r_1, \ldots, r_k > 0$, $\sum_{u=1}^k r_u = 1$. Then $G_n(P, P_k) \to W_H$ as $n \to \infty$, where $H$ is a vertex- and edge-weighted graph on $k$ vertices with vertex-weights $r_1, \ldots, r_k$, the edge-weights are the entries of $P$, and $W_H$ is the stepfunction graphon corresponding to $H$.

In [28] the following definition of a generalized quasirandom graph sequence was given.

**Definition 3.** Given a model graph graph $H$ on $k$ vertices with vertex-weights $r_1, \ldots, r_k$ and edge-weights $p_{uv} = p_{vu}$, $1 \leq u \leq v \leq k$ (entries of $P$), $(G_n)$ is $H$-quasirandom if $G_n \to W_H$ as $n \to \infty$ in terms of the homomorphism densities.

The authors of [28] also proved that the vertex set $V$ of a generalized quasirandom graph $G_n$ can be partitioned into classes $C_1, \ldots, C_k$ in such a way that $\frac{|C_u|}{|V|} \to r_u (u = 1, \ldots, k)$ and the subgraph of $G_n$ induced by $C_u$ is the general term of a quasirandom graph sequence with edge-density tending to $p_{uv}$ (for $u = 1, \ldots, k$), whereas the bipartite subgraph between $C_u$ and $C_v$ is the general term of a quasirandom bipartite graph sequence with edge-density tending to $p_{uv}$ as $n \to \infty$.

Because of the limit relation in the definition of the generalized quasirandom graphs, and the spectral equivalence of convergent graph sequences, the properties, discussed in Proposition 1, are as well valid for the generalized quasirandom graphs. Actually, the authors in [17] proved that for any $k$, the $k$ largest absolute value normalized adjacency eigenvalues of a convergent graph sequence converge (to
the corresponding eigenvalues of the limiting graphon). In [9] we proved the same for the normalized modularity spectra of convergent graph sequences.

How to construct a generalized quasirandom graph with given $k$, $P$, and vertex-weights of the model graph $H$? Consider the instance when there are $k$ clusters $C_1, \ldots, C_k$ of the vertices of sizes $n_1, \ldots, n_k$ such that $\frac{n_u}{n} = r_u (u = 1, \ldots, k)$. Let us choose the independent irrational numbers $\alpha_{uv} (1 \leq u \leq v \leq k)$. Then the subgraph on the vertex-set $C_u$ is constructed as follows: $i, j \in C_u$, $i < j$ are connected if and only if

$$\{(i - j)^2\alpha_{uv}\} < p_{uu} \quad (u = 1, \ldots, k),$$

where $\{\}$ denotes the fractional part of a real number. The bipartite subgraph between $C_u$ and $C_v$ is constructed as follows: $i \in C_u$ and $j \in C_v$ are connected if and only if

$$\{(i - j)^2\alpha_{uv}\} < p_{uv} \quad (1 \leq u < v \leq k).$$

Analytical number theoretical considerations (see, e.g., [13, 32]) guarantee that, for any $1 \leq u \leq v \leq k$, the sequence

$$y_t := \{(t - i)^2\alpha_{uv}\}, \{(t - j)^2\alpha_{uv}\}$$

is well-distributed symmetrically in $[0, 1]^2$, uniformly in $i, j \in C_u (i \neq j)$. Therefore, with the considerations of [32],

$$\left| \left\{ t \in C_v : \{(t - i)^2\alpha_{uv}\} < p_{uv} \right\} \right| \leq p_{uv}^2 n_v + o(n_v) = p_{uv}^2 n_v + o(n)$$

if $n \to \infty$ and $\frac{n_u}{n} \to r_u (u = 1, \ldots, k)$. For more examples of quasirandom graphs in the $k = 1$ case see [12, 13, 36].

Therefore, a large random graph, constructed in this way, will be ‘nearly’ $k$-partite, $k$-regular, and its normalized modularity spectrum contains $k - 1$ structural eigenvalues, whereas, all the other eigenvalues are $o(1)$, akin to the weighted $k$-variance of the optimal $(k - 1)$-dimensional representatives. In this case, the $k$-way discrepancy in the optimal spectral clustering is $o(1)$. As for the complete $k$-partite graph $K_{n_1, \ldots, n_k}$ (pure case), its normalized modularity spectrum contains $k - 1$ structural negative eigenvalues and $n - k + 1$ zeros. Also, the above $k$-variance is zero; further, $\text{disc}_k(K_{n_1, \ldots, n_k}) = 0$ and $s_k = 0$.

For an illustration of generalized random and quasirandom graphs see Figures 1, 2, 3.

$$P = \begin{pmatrix} 0.7 & 0.1 & 0.15 & 0.2 & 0.25 \\ 0.1 & 0.75 & 0.3 & 0.35 & 0.4 \\ 0.15 & 0.3 & 0.8 & 0.45 & 0.5 \\ 0.2 & 0.35 & 0.45 & 0.85 & 0.55 \\ 0.25 & 0.4 & 0.5 & 0.55 & 0.9 \end{pmatrix}$$

The properties of Proposition 1 can be regarded as generalized quasirandom properties provided their implications can be proved for any graph sequence. To make the idea more precise, we formulate the following conjecture.

**Conjecture 1.** Consider the sequence of graphs $G_n$ with vertex-set $V_n$, adjacency matrix $A_n$, and normalized modularity matrix $M_{D,n}$. Let $k$ be a fixed positive integer and $|V_n| = n \to \infty$. Then the following properties are equivalent:

**PI.** (a) $A_n$ has $k$ structural eigenvalues that are $\Theta(n)$ in absolute value, while the remaining eigenvalues are $o(n)$.

(b) The $k$-variance $S_{k,n}^2$ of the $k$-dimensional vertex representatives, based on the eigenvectors corresponding to the structural eigenvalues of $A_n$, is $o(1)$. The $k$-partition $P_k = (C_1, \ldots, C_k)$ minimizing this $k$-variance is such that $\frac{n_u}{n} \geq c$ ($u = 1, \ldots, k$) holds with some constant $c$, where $n_u = |C_u|$.

**PII.** (a) There exists a constant $0 < \delta < 1$ (independent of $n$, it only depends on $k$) such that $M_{D,n}$ has $k - 1$ structural eigenvalues that are greater than $\delta$ in absolute value, while the remaining eigenvalues are $o(1)$. 
(b) The weighted $k$-variance $S_{k,n}^2$ of the $(k-1)$-dimensional vertex representatives, based on the transformed eigenvectors corresponding to the structural eigenvalues of $M_{D,n}$, is $o(1)$. The $k$-partition $P_k = (C_1, \ldots, C_k)$ minimizing the above weighted $k$-variance is such that $\frac{n_u}{n} \geq c$ ($u = 1, \ldots, k$) holds with some constant $c$, where $n_u = |C_u|$.  

**III.** There are vertex-classes $P_k = (C_1, \ldots, C_k)$ of sizes $n_1, \ldots, n_k$, satisfying $\frac{n_u}{n} \geq c$ ($u = 1, \ldots, k$) and a constant $0 < \theta < 1$ (independent of $n$) such that $\text{disc}_1(G_n), \ldots, \text{disc}_{k-1}(G_n) > \theta$, and $\text{disc}_k(G_n; C_1, \ldots, C_k) = o(1)$.  

**IV.** There are vertex-classes $P_k = (C_1, \ldots, C_k)$ of sizes $n_1, \ldots, n_k$, satisfying $\frac{n_u}{n} \geq c$ ($u = 1, \ldots, k$) and a $k \times k$ symmetric probability matrix $P = (p_{uv})$, such that every vertex of $C_u$ has asymptotically $n_u p_{uv}$ neighbors in $C_v$ for any $1 \leq u \leq v \leq k$ pair. Further, for the codegrees (number of common neighbors) the following holds: every two different vertices $i, j \in C_u$ have asymptotically $p_{uv}^2 n_v$ common neighbors in $C_v$ for any $1 \leq u \leq v \leq k$ pair. More exactly, for every $1 \leq u \leq v \leq k$ and $i, j \in C_u$:  

$$\sum_{t \in C_v} a_{it} = p_{uv} n_v + o(n);$$  

and for every $1 \leq u \leq v \leq k$ and $i, j \in C_u$:  

$$\sum_{t \in C_v} a_{it} a_{jt} = p_{uv}^2 n_v + o(n).$$  

The PI-PII implications follow from the statements of Chapter 3 [8]. Particularly, statement (a) implies (b) by subspace perturbation theorems both in PI and PII. The PII→PIII implication is proved in [9], 10 and discussed in Section 4. As for the PIII→PII implication, we will prove Theorem 1 in Section 4. Based on the results of [19, 37] we guess that PIII implies PIV, and vice versa. With some transformation, theorems of [36, 37] about $(p, \alpha)$-jumbled graphs may be applicable for the subgraphs and bipartite subgraphs, where $p$ is some $p_{uv}$ and $\alpha$ is related to the $k$-way discrepancy.
4 Discrepancy versus spectra

Here we extend the notion of discrepancy to rectangular matrices of nonnegative entries, like microarrays or contingency tables. Edge-weighted and directed graphs are special cases.

Let \( A = (a_{ij}) \) be an \( m \times n \) matrix with \( a_{ij} \geq 0 \). We assume that \( AA^T \) (when \( m \leq n \)) or \( A^TA \) (when \( m > n \)) is irreducible. Consequently, the row-sums \( d_{row,i} = \sum_{j=1}^n a_{ij} \) and column-sums \( d_{col,j} = \sum_{i=1}^m a_{ij} \) of \( A \) are strictly positive, and the diagonal matrices \( D_{row} = \text{diag}(d_{row,1}, \ldots, d_{row,m}) \) and \( D_{col} = \text{diag}(d_{col,1}, \ldots, d_{col,n}) \) are invertible. Without loss of generality, we mostly assume that \( \sum_{i=1}^m \sum_{j=1}^m a_{ij} = 1 \), since the normalized table \( A_D = D_{row}^{-1/2} A D_{col}^{-1/2} \),

\[
\text{(6)}
\]

is not affected by the scaling of the entries of \( A \). It is well known (see e.g., [10]) that the singular values of \( A_D \) are in the \([0,1]\) interval. Enumerated in non-increasing order, the positive ones are the real numbers

\[
1 = s_0 > s_1 \geq \cdots \geq s_r - 1 > 0,
\]

where \( r = \text{rank}(A) \). Under the above conditions, 1 is a single singular value, and it is denoted by \( s_0 \), since it belongs to the trivial singular vector pair. In [10] we estimated the multiway discrepancy, to be introduced, of \( A \) by means of these singular values and the corresponding spectral subspaces.

**Definition 4.** The multiway discrepancy of the rectangular array \( A \) of nonnegative entries in the proper \( k \)-partition \( R_1, \ldots, R_k \) of its rows and \( C_1, \ldots, C_k \) of its columns is

\[
\text{disc}(A; R_1, \ldots, R_k, C_1, \ldots, C_k) = \max_{1 \leq u, v \leq k} \max_{X \subseteq R_u, Y \subseteq C_v} \text{disc}(X, Y; R_u, C_v),
\]

\[
\text{(7)}
\]

where

\[
\text{disc}(X, Y; R_u, C_v) = \frac{|a(X, Y) - \rho(R_u, C_v) \text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}}
\]

\[
= |\rho(X, Y) - \rho(R_u, C_v)| \sqrt{\text{Vol}(X)\text{Vol}(Y)}.
\]

\[
\text{(8)}
\]

Here \( a(X, Y) = \sum_{i \in X} \sum_{j \in Y} a_{ij} \) is the cut between \( X \subseteq R_u \) and \( Y \subseteq C_v \), \( \text{Vol}(X) = \sum_{i \in X} d_{row,i} \) is the volume of the row-subset \( X \), \( \text{Vol}(Y) = \sum_{j \in Y} d_{col,j} \) is the volume of the column-subset \( Y \), whereas \( \rho(X, Y) = \frac{a(X, Y)}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}} \) denotes the density between \( X \) and \( Y \). The minimum \( k \)-way discrepancy of \( A \) is

\[
\text{disc}_k(A) = \min_{R_1, \ldots, R_k, C_1, \ldots, C_k} \text{disc}(A; R_1, \ldots, R_k, C_1, \ldots, C_k).
\]

In [10], we proved that given the \( m \times n \) rectangular array \( A \), the following spectral biclustering results in row-column cluster pairs of small discrepancy. The clusters \( R_1, \ldots, R_k \) of the rows and \( C_1, \ldots, C_k \) of the columns are obtained by applying the weighted \( k \)-means algorithm for the \((k - 1)\)-dimensional row- and column representatives, defined as the row vectors of the matrices of column vectors \( (D_{row}^{-1/2}v_1, \ldots, D_{row}^{-1/2}v_{k-1}) \) and \( (D_{col}^{-1/2}u_1, \ldots, D_{col}^{-1/2}u_{k-1}) \), respectively, where \( v_i, u_i \) is the unit norm singular vector pair corresponding to \( s_i \) (\( i = 1, \ldots, k - 1 \)). Recall that these partitions minimize the weighted \( k \)-variances \( S_{k,row}^2 \) and \( S_{k,col}^2 \) of these row- and column-representatived introduced in (4). Then, under some balancing conditions for the margins and for the cluster sizes, we proved that \( \text{disc}_k(A) = O(\sqrt{2k} \cdot S_{k,row} + S_{k,col} + s_k) \).

In the special case when \( m = n \) and \( A \) is symmetric of zero diagonal, we have the edge-weight matrix of an undirected graph. In [9], we proved the following for the \( k \)-way discrepancy of the edge-weighted graph \( G = (V, A_n) \), where the singular values of \( M_{D,n} \) are the numbers \( s_i = |\mu_i| \) (\( i = 1, \ldots, n \)).

**Proposition 4.** Let \( G = (V, W) \) be a connected edge-weighted graph on \( n \) vertices, with generalized degrees \( d_1, \ldots, d_n \) and degree matrix \( D \). Assume that \( \text{Vol}(V) = 1 \), and there are no dominant vertices,
Let the eigenvalues of $M_{D,n}$, enumerated in decreasing absolute values, be

$$1 \geq |\mu_1| \geq \cdots \geq |\mu_{k-1}| > \varepsilon \geq |\mu_k| \geq \cdots \geq |\mu_n| = 0.$$  

The partition \((C_1, \ldots, C_k)\) of \(V\) is defined so that it minimizes the weighted \(k\)-variance \(S_k^2\) of the optimum vertex representatives obtained as row vectors of the \(n \times (k-1)\) matrix of column vectors \(D_n^{-1/2}u_{i,n}\), where \(u_{i,n}\) is the unit-norm eigenvector corresponding to \(\mu_{i,n}\) (\(i = 1, \ldots, k-1\)). Assume that there is a constant \(0 < K \leq \frac{1}{2}\) such that \(|C_i| \geq Kn\), \(i = 1, \ldots, k\). With the notation \(s = \sqrt{S_k^2}\), the \((C_i, C_j)\) pairs are \(O(\sqrt{2k}s + \varepsilon)\)-volume regular \((i \neq j)\) and for the clusters \(C_i\) \((i = 1, \ldots, k)\) the following holds: for all \(X,Y \subset V_i\),

$$|w(X,Y) - \rho(C_i)\Vol(X)\Vol(Y)| = O(\sqrt{2k}s + \varepsilon)\Vol(C_i),$$

where \(\rho(C_i) = \frac{w(V_i, V_i)}{\Vol(V_i)}\) is the relative intra-cluster density of \(C_i\).

Then, by Proposition 4, PII implies PIII, under some balancing conditions for the margins and for the cluster sizes. Conversely, we are able to estimate \(s_k\) with the \(k\)-way discrepancy.

**Theorem 1.** With the above notation,

$$s_k = O(\sqrt{\log m \log n})$$

for any positive integer \(k < \text{rank}(A)\).

For the proof we need the following lemmas. Lemma 3 of Bollobás and Nikiforov [14] states that to every \(0 < \varepsilon < 1\) and vector \(x \in \mathbb{C}^n\), \(\|x\| = 1\), there exists a vector \(y \in \mathbb{C}^n\) such that its coordinates take no more than \(\left\lceil \frac{n}{\varepsilon} \right\rceil \left\lceil \frac{1}{2 \log n} \right\rceil\) distinct values and \(\|x - y\| \leq \varepsilon\). Lemma 3 of Butler [18] can be traced back to this one. It states that to any vector \(x \in \mathbb{C}^n\), \(\|x\| = 1\) and diagonal matrix \(D\) of positive real diagonal entries, one can construct a step-vector \(y \in \mathbb{C}^n\) such that \(\|x - Dy\| \leq \frac{1}{2}, \|Dy\| \leq 1\), and \(y\) has at most \(\Theta(\log n)\) distinct coordinates. We well also use the following lemma that we constructed just 10 for this purpose.

**Lemma 2.** Let \(A\) be an \(m \times n\) matrix of real entries and let the rows and columns have positive real weights \(d_{i,j}\)'s and \(d_{c,j}\)'s (independently of the entries of \(A\)), which are collected in the main diagonals of the \(m \times m\) and \(n \times n\) diagonal matrices \(D_r\) and \(D_c\), respectively. Let \(R_1, \ldots, R_k\) and \(C_1, \ldots, C_l\) be proper partitions of the rows and columns; further, \(x \in \mathbb{C}^m\) and \(y \in \mathbb{C}^n\) be stepwise constant vectors having equal coordinates over the index sets corresponding to the partition members of \(R_1, \ldots, R_k\) and \(C_1, \ldots, C_l\), respectively. The \(k \times \ell\) real matrix \(A' = (a'_{u,v})\) is defined by

$$a'_{u,v} := \frac{a(R_u, C_v)}{\Vol(R_u)\Vol(C_v)}, \quad u = 1, \ldots, k; \quad v = 1, \ldots, \ell,$$

where \(a(R_u, C_v)\) is the usual cut of \(A\) between \(R_u\) and \(C_v\), whereas \(\Vol(R_u) = \sum_{i \in R_u} d_{r,i}\) and \(\Vol(C_v) = \sum_{j \in C_v} d_{c,j}\). Then

$$\|(x, Ay)\| \leq \|A'\| \cdot \|D_r^{1/2}x\| \cdot \|D_c^{1/2}y\|,$$

where \(\|A'\|\) denotes the spectral norm, that is the largest singular value of the real matrix \(A'\), and the squared norm of a complex vector is the sum of the squares of the absolute values of its coordinates.

Note that here the row- and column-weights have nothing to do with the entries of \(A\), and the volumes are usually not the ones defined in Section 2; this is why they are denoted by \(\Vol\) instead of \(\text{Vol}\).

**Proof of Lemma 2.** For the distinct coordinates of \(x\) and \(y\) we introduce

$$x_i := \frac{x'_i}{\sqrt{\Vol(R_u)}} \quad \text{if} \quad i \in R_u \quad \text{and} \quad y_j := \frac{y'_j}{\sqrt{\Vol(C_b)}} \quad \text{if} \quad j \in C_b$$
with \( x'_a \) and \( y'_b \) that are coordinates of \( x' \in \mathbb{C}^k \) and \( y' \in \mathbb{C}^l \). Obviously, \( \| D_{x'}^k x \| = \| x' \| \) and \( \| D_{y'}^l y \| = \| y' \| \). Then, using \( -\) for the complex conjugation,

\[
\langle x, Ay \rangle = \sum_{i=1}^m \sum_{j=1}^n x_i y_j c_{ij} = \sum_{a=1}^k \sum_{b=1}^l x'_a y'_b \frac{c(R_a, C_b)}{\text{VOL}(R_a)} \frac{c(R_a, C_b)}{\text{VOL}(C_b)}
\]

\[
= \sum_{a=1}^k \sum_{b=1}^l x'_a y'_b c_{ab} = \langle x', A' y' \rangle \leq s_{\text{max}}(A') \cdot \| x' \| \cdot \| y' \|
\]

by the well-known extremal property of the largest singular value, which finishes the proof.

**Proof of Theorem 1.** Assume that \( \alpha = \text{disc}_k(A) \) is attained with the proper \( k \)-partition \( R_1, \ldots, R_k \) of the rows and \( C_1, \ldots, C_k \) of the columns of \( A \); i.e., for every \( R_a, C_b \) pair and \( X \subset R_a, Y \subset C_b \) we have

\[
|c(X, Y) - \rho(R_a, C_b)\text{Vol}(X)\text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(X)\text{Vol}(Y)}.
\]

Introducing the \( m \times n \) matrix

\[
F = A - D_{\text{row}}RD_{\text{col}},
\]

where \( R = (\rho(R_a, C_b)) \) is the \( m \times n \) block-matrix of \( k \times k \) blocks with entries equal to \( \rho(R_a, C_b) \) over the block \( R_u \times C_v \), Equation (10) yields

\[
D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} = D_{\text{row}}^{-1/2}A D_{\text{col}}^{-1/2} - D_{\text{row}}^{-1/2}RD_{\text{col}}^{-1/2} = A_D - D_{\text{row}}^{-1/2}RD_{\text{col}}^{-1/2}.
\]

Since the rank of the matrix \( D_{\text{row}}^{-1/2}RD_{\text{col}}^{-1/2} \) is at most \( k \), by Theorem 3 of Thompson [38], describing the effect of rank \( k \) perturbations for the singular values, we obtain the following upper estimate for \( s_k \), that is the \((k+1)\)th largest (including the trivial 1) singular value of \( A_D \):

\[
s_k \leq s_{\text{max}}(D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2}) = \| D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} \|,
\]

where \( \| . \| \) denotes the spectral norm.

Let \( v \in \mathbb{R}^m \) be the left and \( u \in \mathbb{R}^n \) be the right unit-norm singular vector corresponding to the maximal singular value of \( D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} \), i.e.,

\[
|\langle v, (D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2})u \rangle| = \| D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} \|.
\]

In view of Butler [18], there are stepwise constant vectors \( x \in \mathbb{C}^m \) and \( y \in \mathbb{C}^n \) such that \( \| v - D_{\text{row}}^{-1/2}x \| \leq \frac{1}{4}, \| u - D_{\text{col}}^{-1/2}y \| \leq \frac{1}{4}, \| D_{\text{row}}^{-1/2}x \| \leq 1, \| D_{\text{col}}^{-1/2}y \| \leq 1 \); further,

\[
\| D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} \| \leq \frac{9}{2} \left\| \left( D_{\text{row}}^{-1/2}x, D_{\text{col}}^{-1/2}y \right) \right\| = \frac{9}{2} \| (x, Fy) \|.
\]

Then, using the above discussed argument and Butler’s results, with the matrix \( F \) defined in (10) and the constructed step-vectors \( x \in \mathbb{C}^m, y \in \mathbb{C}^n \), we have

\[
s_k \leq \| D_{\text{row}}^{-1/2}F D_{\text{col}}^{-1/2} \| \leq \frac{9}{2} \| (x, Fy) \|
\]

With the preliminary argument, \( x \) takes on at most \( r_1 = \Theta(\log m) \), and \( y \) takes on at most \( r_2 = \Theta(\log n) \) distinct values, which define the proper partitions \( P_1, \ldots, P_{r_1} \) of the rows and \( Q_1, \ldots, Q_{r_2} \) of the columns. Let us consider the subdivision of them with respect to \( R_1, \ldots, R_k \) and \( C_1, \ldots, C_k \). In this way, we obtain the proper partition \( P'_1, \ldots, P'_\ell_1 \) of the rows and \( Q'_1, \ldots, Q'_\ell_2 \) of the columns with at most \( \ell_1 \) \( r_1 \) and \( \ell_2 \) \( r_2 \) parts.

Now, we apply Lemma 2 to the matrix \( F \) and to the step-vectors \( x \) and \( y \), which are also stepwise constant with respect to the above partitions. The row-weights and column-weights are the \( d_{\text{row},i} \)'s and \( d_{\text{col},j} \)'s, respectively. In view of the lemma, the entries of the \( \ell_1 \times \ell_2 \) matrix \( F' \) are

\[
f'_{uv} := \frac{f(P'_u, Q'_v)}{\sqrt{\text{Vol}(P'_u)\text{Vol}(Q'_v)}}
\]
Matrices of generalized random graphs

and

$$|⟨x, Fy⟩| ≤ ∥F'∥ · ∥D^{1/2}_{row}x∥ · ∥D^{1/2}_{col}y∥ ≤ ∥F'∥.$$  

But by a well-known linear algebra fact we get that

$$∥F'∥ = s_{max}(F') ≤ \sqrt{\ell_1 \ell_2} \max_{u \in [\ell_1]} \max_{v \in [\ell_2]} |f'_{uv}| ≤ \ell \cdot \text{disc}(A; R_1, \ldots, R_k, C_1, \ldots, C_k),$$

where $\ell = \sqrt{\ell_1 \ell_2}$ and we used Formula (7) for the discrepancy. Consequently,

$$s_k ≤ \frac{9}{2} \ell \text{disc}_k(A)$$

follows.

Note that, by Theorem 1, for the undirected, edge-weighted graph $G_n$, the relation $|\mu_k| = O(\log n) \text{disc}_k(G_n)$ holds; therefore, if in addition $\text{disc}_k(G_n) = O(n^{-\tau})$ with some $0 < \tau < \frac{1}{2}$, as in the case of generalized random and quasirandom graphs, then PIII implies PII.

The discrepancy of a directed graph $G = (V, W)$ is a special case of that of a rectangular array in that its edge-weight matrix $W = (w_{ij})$ is quadratic, but asymmetric: $w_{ij} ≥ 0$ is the weight of the $i \rightarrow j$ edge $(i \neq j)$ and $w_{ii} = 0$ ($i = 1, \ldots, n$). We used the spectral clustering algorithm to migration data between 34 countries. The row- and column-clusters are the out- and in-clusters, corresponding to countries exhibiting similar emigration and immigration patterns; $w_{ij}$ represents the number of persons in thousands who moved from country $i$ to country $j$ during the year 2011.

Based on the singular values

$$s_0 = 1, s_1 = 0.79067, s_2 = 0.769678, s_3 = 0.61489, s_4 = 0.584317, s_5 = 0.56072, \ldots, s_{33} = 0.000523946$$

of the normalized (asymmetric) $34 \times 34$ edge-weight matrix $W_D$, there was indeed a gap after $s_2$, so we found three clusters for both the rows and the columns. The row-clusters (emigration trait clusters) were the following:

1. Australia, Austria, Canada, Chile, Czech Republic, Estonia, Greece, Hungary, Israel, Japan, Korea, Luxembourg, Mexico, New Zealand, Poland, Slovak Republic, Slovenia, Turkey, United States.
2. Belgium, France, Germany, Ireland, Italy, Netherlands, Portugal, Spain, Switzerland, United Kingdom.
3. Denmark, Finland, Iceland, Norway, Sweden.

The clusters (immigration trait clusters) were:

1. Australia, Austria, Belgium, France, Greece, Israel, Italy, Luxembourg, Poland, Portugal, Spain, Switzerland, United Kingdom.
2. Canada, Chile, Czech Republic, Germany, Hungary, Iceland, Ireland, Japan, Korea, Mexico, Netherlands, New Zealand, Slovak Republic, Slovenia, Turkey, United States.
3. Denmark, Estonia, Finland, Norway, Sweden.

Figure 4 shows the results, where we can spot some dense and sparse edge-densities within the subgraphs and bipartite subgraphs. For example, there is a high edge-density between out-cluster 2 and in-cluster 1, which indicates frequent migration between the countries of the European Union. Also, high edge-density is shown between out-cluster 3 and in-cluster 3, i.e., between the countries of Northern Europe, in 2011. However, their separation is not so spectacular, since with $n = 34$ the asymptotic properties are not clearly effectuated.

5 Conclusion

We characterized spectra and discrepancies of generalized random and quasirandom graphs. Properties, like ‘large’ spectral gap, ‘small’ within-cluster variances of the vertex representatives, and ‘small’ within- and between-cluster discrepancies were formulated with graph based matrices, for a given number of clusters. However, our theory helps the practitioners to find the optimal number of clusters.
As a generalization of quasirandomness, that applies to the one-cluster situation, we also considered
generalized quasirandom properties, and proved some implications between them, irrespective of stochas-
tic models. Real-life expanding graph sequences asymptotically capturing one of these properties are
random-like, confined to the subgraphs and bipartite subgraphs of them. The equivalences also suggest
that spectral methods are capable to find partitions of the vertices with ‘small’ multiway discrepancy.
We extended these notions to rectangular arrays of nonnegative entries, of which directed graphs are
special cases.

Acknowledgements

The authors wish to thank Vera T. Sós and Gergely Kiss for useful advises on the quasirandom graph
construction.

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