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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 5
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 10
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

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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 20
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 $G_n(\mathbf{P}, \mathcal{P}_k)$ on n vertices is a generalized random graph with $k \times k$ symmetric *probability*
matrix $\mathbf{P} = (p_{uv})$ and proper k -partition $\mathcal{P}_k = (C_1, \dots, C_k)$ of the vertices ($|C_u| = n_u$) if vertices of 25
 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} ($u = 1, \dots, k$). Therefore, the subgraph of
 $G_n(\mathbf{P}, \mathcal{P}_k)$ 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, \dots, C_k are the clusters. 30

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 $G_n(\mathbf{P}, \mathcal{P}_k)$ as $n \rightarrow \infty$ 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 $o(1)$. 35
The k -way discrepancy of $G_n(\mathbf{P}, \mathcal{P}_k)$ also tends to 0, and the subgraphs and bipartite subgraphs defined

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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 $G = (V, \mathbf{W})$ be an *edge-weighted graph* on the n -element vertex-set V with the $n \times n$ symmetric weight-matrix \mathbf{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 $\mathbf{M} = \mathbf{W} - \mathbf{d}\mathbf{d}^T$, where the entries of \mathbf{d} are the *generalized vertex-degrees* $d_i = \sum_{j=1}^n w_{ij}$ ($i = 1, \dots, n$). Here \mathbf{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 \mathbf{W} :

$$\mathbf{M}_D = \mathbf{D}^{-1/2} \mathbf{M} \mathbf{D}^{-1/2},$$

where $\mathbf{D} = \text{diag}(d_1, \dots, d_n)$ 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 \mathbf{W} being *irreducible*, in which case, the generalized vertex-degrees are all positive. The modularity matrix \mathbf{M} always has a zero eigenvalue with eigenvector $\mathbf{1}_n = (1, \dots, 1)^T$, since its rows sum to zero. Because of $\text{tr}(\mathbf{M}) < 0$, \mathbf{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 \mathbf{M}_D are in the $[-1, 1]$ interval, and 1 cannot be an eigenvalue if G is connected. \mathbf{M}_D is closely related to the *normalized Laplacian* matrix. The *normalized Laplacian* of $G = (V, \mathbf{W})$ is defined as $\mathbf{L}_D = \mathbf{I} - \mathbf{D}^{-1/2} \mathbf{W} \mathbf{D}^{-1/2}$, and the following relation can be established between the spectra of \mathbf{L}_D and \mathbf{M}_D when G is connected. Let $0 = \lambda_0 < \lambda_1 \leq \dots \leq \lambda_{n-1} \leq 2$ denote the eigenvalues of \mathbf{L}_D . The zero is a single eigenvalue with corresponding unit-norm eigenvector $\sqrt{\mathbf{d}} := (\sqrt{d_1}, \dots, \sqrt{d_n})^T$. The eigenvalues of \mathbf{M}_D are the numbers $1 - \lambda_i$ with the same eigenvectors ($i = 1, \dots, n-1$); further, the zero with corresponding unit-norm eigenvector $\sqrt{\mathbf{d}}$.

Let $1 < k < n$ be a fixed integer. Usual spectral clustering techniques use the k bottom eigenvalues $\lambda_0, \dots, \lambda_{k-1}$ of \mathbf{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, \dots, 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 \mathbf{M} is $w_{ij} - d_i d_j$, 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

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

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 $\rho(X, Y) := \frac{w(X, Y)}{\text{Vol}(X) \text{Vol}(Y)}$ be the density between X and Y .

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

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

where

$$\begin{aligned} \text{disc}(X, Y; C_u, C_v) &= \frac{|w(X, Y) - \rho(C_u, C_v) \text{Vol}(X) \text{Vol}(Y)|}{\sqrt{\text{Vol}(X) \text{Vol}(Y)}} \\ &= |\rho(X, Y) - \rho(C_u, C_v)| \sqrt{\text{Vol}(X) \text{Vol}(Y)}. \end{aligned} \quad (2)$$

The minimum k -way discrepancy of G is

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

Note that $\text{disc}(G; C_1, \dots, C_k)$ is the smallest α 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 α -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 ϵ -regular pairs in the Szemerédi regularity lemma [35], albeit with given number of vertex-clusters, which are usually not
 5 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 $1 > |\mu_1| \geq |\mu_2| \geq \dots \geq |\mu_n| = 0$. Assume that $|\mu_{k-1}| > |\mu_k|$, and denote by $\mathbf{u}_1, \dots, \mathbf{u}_{k-1}$ the corresponding unit-norm, pairwise orthogonal eigenvectors. Let $\mathbf{r}_1, \dots, \mathbf{r}_n \in \mathbb{R}^{k-1}$ be the row vectors of the $n \times (k-1)$
 10 matrix of column vectors $\mathbf{D}^{-1/2}\mathbf{u}_1, \dots, \mathbf{D}^{-1/2}\mathbf{u}_{k-1}$; they are called $(k-1)$ -dimensional representatives of the vertices.

The *weighted k -variance* of these representatives is defined as

$$\tilde{S}_k^2 = \min_{(C_1, \dots, C_k)} \sum_{u=1}^k \sum_{j \in C_u} d_j \|\mathbf{r}_j - \mathbf{c}_u\|^2, \quad (4)$$

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
 15 between the eigensubspace corresponding to μ_0, \dots, μ_{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
 20 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 $\mathbf{r}_1, \dots, \mathbf{r}_n \in \mathbb{R}^k$ 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

$$S_k^2 = \min_{(C_1, \dots, C_k)} \sum_{u=1}^k \sum_{j \in C_u} \|\mathbf{r}_j - \mathbf{c}_u\|^2, \quad (5)$$

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
 25 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 and the
 30 ‘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 $\mathcal{P}_k = (C_1, \dots, C_k)$ 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
 35 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} ($u = 1, \dots, k$).

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 $G_n(p)$. 5

Note that that Definition 2 makes sense if the probability matrix \mathbf{P} contains at least one non-zero entry. In many cases, one or more entries of \mathbf{P} are zeros. In particular, when $p_{uu} = 0$ ($u = 1, \dots, k$) and $p_{uv} = p \in (0, 1)$, then the graph $G_n(\mathbf{P}, \mathcal{P}_k)$ 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, \dots, n_k} over the independent vertex classes of \mathcal{P}_k , where $n_i = |C_i|$ ($i = 1, \dots, k$). 10

If $k = n$ and $p_{ij} := d_i d_j / \sum_{m=1}^n d_m$ ($i, j = 1, \dots, n$), then the model gives the random graph with expected degree sequence d_1, \dots, 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 [3], 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 \mathbf{P} fixed, while $n \rightarrow \infty$ under some balancing conditions on the cluster sizes. In [5, 6, 8] we proved the following properties of a generalized random graph. 15

Proposition 1. *Let $G_n(\mathbf{P}, \mathcal{P}_k)$ be a generalized random graph on n vertices with vertex-classes $\mathcal{P}_k = (C_1, \dots, C_k)$ of sizes n_1, \dots, n_k and $k \times k$ symmetric probability matrix \mathbf{P} . Let k be a fixed positive integer and $n \rightarrow \infty$ in such a way that $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) with some constant $0 < c \leq \frac{1}{k}$ (called balancing condition). Then the following hold almost surely for the adjacency matrix \mathbf{A}_n and the normalized modularity matrix $\mathbf{M}_{D,n}$ of $G_n(\mathbf{P}, \mathcal{P}_k)$. 20*

1. \mathbf{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 \mathbf{A}_n (see (5)), is $O(\frac{1}{n})$. 25
2. There exists a positive constant $0 < \delta < 1$ independent of n (it only depends on k) such that $\mathbf{M}_{D,n}$ has exactly $k-1$ structural eigenvalues of absolute value greater than δ , 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 $\tilde{S}_{k,n}^2$ of the $(k-1)$ -dimensional vertex representatives, based on the transformed eigenvectors corresponding to the structural eigenvalues of $\mathbf{M}_{D,n}$ (see (4)), is $O(n^{-\tau})$. 30
3. There is a constant $0 < \theta < 1$ (independent of n) such that $\text{disc}_1(G_n(\mathbf{P}, \mathcal{P}_k)) > \theta, \dots, \text{disc}_{k-1}(G_n(\mathbf{P}, \mathcal{P}_k)) > \theta$, and the k -way discrepancy $\text{disc}_k(G_n(\mathbf{P}, \mathcal{P}_k); C_1, \dots, C_k)$ 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 $i, j \in C_u$:

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

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. 35

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

$$\mathbb{P}(|X - \mathbb{E}(X)| > a) \leq e^{-\frac{a^2}{2(\text{Var}(X) + Ka/3)}}.$$

Proof of Property 4. Consider the generalized random graph sequence $G_n(\mathbf{P}, \mathcal{P}_k)$, the subgraphs and the bipartite subgraphs of which have the following expected degrees. We will drop the index n , and use

the notation $\mathbf{A} = (a_{ij})$ 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

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

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 $n \rightarrow \infty$ under the balancing conditions $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) for the cluster sizes. Indeed, for any $0 < \varepsilon < 1$:

$$\mathbb{P}\left(\left|\frac{1}{n_v} \sum_{j \in C_v} a_{ij} - p_{uv}\right| > \varepsilon\right) = \mathbb{P}\left(\left|\sum_{j \in C_v} a_{ij} - n_v p_{uv}\right| > n_v \varepsilon\right) \leq e^{-\frac{n_v^2 \varepsilon^2}{2(n_v p_{uv}(1-p_{uv}) + \varepsilon/3)}}$$

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

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

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 bipar-
5 tite 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
10 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 $1 - \|\mathbf{M}_D\|$. This relation is summarized in the following proposition that is a straightforward generalization of the
15 *Expander Mixing Lemma for irregular graphs*.

Proposition 2.

$$\text{disc}(G) = \text{disc}_1(G) \leq \|\mathbf{M}_D\| = |\mu_1|,$$

where $\|\mathbf{M}_D\|$ 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 \mathbf{M}_D is the maximum of the bilinear form $\mathbf{v}^T \mathbf{M}_D \mathbf{u}$ over the unit sphere. Let $X, Y \subset V$ be arbitrary, and denote by $\mathbf{1}_X, \mathbf{1}_Y \in \mathbb{R}^n$ the indicator vectors of them. Then

$$\begin{aligned} \|\mathbf{M}_D\| &= \max_{\|\mathbf{u}\|=\|\mathbf{v}\|=1} |\mathbf{v}^T \mathbf{M}_D \mathbf{u}| \geq \left| \left(\frac{\mathbf{D}^{1/2} \mathbf{1}_X}{\|\mathbf{D}^{1/2} \mathbf{1}_X\|} \right)^T \mathbf{M}_D \left(\frac{\mathbf{D}^{1/2} \mathbf{1}_Y}{\|\mathbf{D}^{1/2} \mathbf{1}_Y\|} \right) \right| \\ &= \frac{|\mathbf{1}_X^T \mathbf{M}_D \mathbf{1}_Y|}{\|\mathbf{D}^{1/2} \mathbf{1}_X\| \cdot \|\mathbf{D}^{1/2} \mathbf{1}_Y\|} = \frac{|w(X, Y) - \text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)}\sqrt{\text{Vol}(Y)}}. \end{aligned}$$

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 the generalized random graphs. Much earlier, in [34] the authors established valuable relations between 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 $n \rightarrow \infty$. They also define the limit object that is a symmetric, bounded, measurable function $W : [0, 1] \times [0, 1] \rightarrow \mathbb{R}$, 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, \dots, 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 $G_n(\mathbf{P}, \mathcal{P}_k)$ with $\mathcal{P}_k = (C_1, \dots, C_k)$, $|C_u| = n_u$ ($u = 1, \dots, k$). Let $n \rightarrow \infty$ in such a way that $\frac{n_u}{n} \rightarrow r_u$ with some $r_1, \dots, r_k > 0$, $\sum_{u=1}^k r_u = 1$. Then $G_n(\mathbf{P}, \mathcal{P}_k) \rightarrow W_H$ as $n \rightarrow \infty$, where H is a vertex- and edge-weighted graph on k vertices with vertex-weights r_1, \dots, r_k , the edge-weights are the entries of \mathbf{P} , and W_H is the step-function graphon corresponding to H .*

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

Definition 3. *Given a model graph H on k vertices with vertex-weights r_1, \dots, r_k and edge-weights $p_{uv} = p_{vu}$, $1 \leq u \leq v \leq k$ (entries of \mathbf{P}), (G_n) is H -quasirandom if $G_n \rightarrow W_H$ as $n \rightarrow \infty$ 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, \dots, C_k in such a way that $\frac{|C_u|}{|V|} \rightarrow r_u$ ($u = 1, \dots, k$) 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_{uu} ($u = 1, \dots, k$), 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} ($u \neq v$) as $n \rightarrow \infty$.

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 , \mathbf{P} , and vertex-weights of the model graph H ? Consider the instance when there are k clusters C_1, \dots, C_k of the vertices of sizes n_1, \dots, n_k such that $\frac{n_u}{n} = r_u$ ($u = 1, \dots, k$). Let us choose the independent irrational numbers α_{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

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

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],

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

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

- 5 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, \dots, n_k} (pure case), its normalized modularity spectrum contains $k - 1$ structural negative eigenvalues
- 10 and $n - k + 1$ zeros. Also, the above k -variance is zero; further, $\text{disc}_k(K_{n_1, \dots, n_k}) = 0$ and $s_k = 0$.

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

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

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.

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

- PI.** (a) \mathbf{A}_n has k structural eigenvalues that are $\Theta(n)$ in absolute value, while the remaining eigenvalues are $o(n)$.
- 20 (b) The k -variance $S_{k,n}^2$ of the k -dimensional vertex representatives, based on the eigenvectors corresponding to the structural eigenvalues of \mathbf{A}_n , is $o(1)$. The k -partition $\mathcal{P}_k = (C_1, \dots, C_k)$ minimizing this k -variance is such that $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) 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 $\mathbf{M}_{D,n}$
- 25 has $k - 1$ structural eigenvalues that are greater than δ in absolute value, while the remaining eigenvalues are $o(1)$.

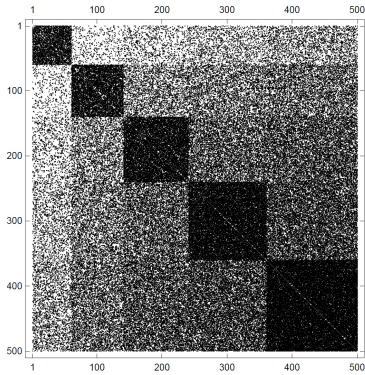


Fig. 1. Generalized random graph generated with $k = 5$, cluster sizes 60, 80, 100, 120, 140 and probability matrix \mathbf{P} below. The first non-trivial eigenvalues of \mathbf{A}_D are 0.304, 0.214, 0.17, 0.153, -0.097 , -0.094 , -0.093 , -0.092 , $-0.091, \dots$, with a gap after the 4th one.

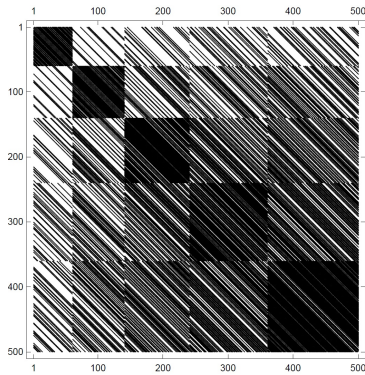


Fig. 2. Generalized quasirandom graph constructed with $k = 5$, cluster sizes 60, 80, 100, 120, 140 and probability matrix \mathbf{P} below. The first non-trivial eigenvalues of \mathbf{A}_D are 0.318, 0.207, 0.154, 0.115, -0.100 , -0.099 , -0.091 , -0.090 , 0.084, \dots , exhibiting decreasing eigenvalues up to the 4th one.

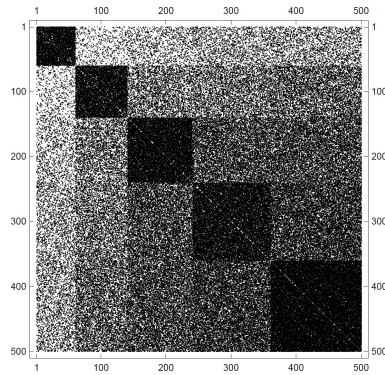


Fig. 3. The former generalized quasirandom graph obtained by appropriate permutation of the vertices within the blocks.

(b) The weighted k -variance $\tilde{S}_{k,n}^2$ of the $(k-1)$ -dimensional vertex representatives, based on the transformed eigenvectors corresponding to the structural eigenvalues of $\mathbf{M}_{D,n}$, is $o(1)$. The k -partition $\mathcal{P}_k = (C_1, \dots, C_k)$ minimizing the above weighted k -variance is such that $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) holds with some constant c , where $n_u = |C_u|$.

PIII. There are vertex-classes $\mathcal{P}_k = (C_1, \dots, C_k)$ of sizes n_1, \dots, n_k , satisfying $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) 5 and a constant $0 < \theta < 1$ (independent of n) such that $\text{disc}_1(G_n), \dots, \text{disc}_{k-1}(G_n) > \theta$, and $\text{disc}_k(G_n; C_1, \dots, C_k) = o(1)$.

PIV. There are vertex-classes $\mathcal{P}_k = (C_1, \dots, C_k)$ of sizes n_1, \dots, n_k , satisfying $\frac{n_u}{n} \geq c$ ($u = 1, \dots, k$) and a $k \times k$ symmetric probability matrix $\mathbf{P} = (p_{uv})$, such that every vertex of C_u has asymptotically $n_v p_{uv}$ 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, α) -jumbled graphs may be applicable for the subgraphs and bipartite subgraphs, where p is some p_{uv} and α 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 $\mathbf{A} = (a_{ij})$ be an $m \times n$ matrix with $a_{ij} \geq 0$. We assume that $\mathbf{A}\mathbf{A}^T$ (when $m \leq n$) or $\mathbf{A}^T\mathbf{A}$ (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 \mathbf{A} are strictly positive, and the diagonal matrices $\mathbf{D}_{row} = \text{diag}(d_{row,1}, \dots, d_{row,m})$ and $\mathbf{D}_{col} = \text{diag}(d_{col,1}, \dots, d_{col,n})$ are invertible. Without loss of generality, we mostly assume that $\sum_{i=1}^m \sum_{j=1}^n a_{ij} = 1$, since the normalized table

$$\mathbf{A}_D = \mathbf{D}_{row}^{-1/2} \mathbf{A} \mathbf{D}_{col}^{-1/2}, \quad (6)$$

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

$$1 = s_0 > s_1 \geq \dots \geq s_{r-1} > 0,$$

where $r = \text{rank}(\mathbf{A})$. 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 \mathbf{A} by means of these singular values and the corresponding spectral subspaces.

Definition 4. The multiway discrepancy of the rectangular array \mathbf{A} of nonnegative entries in the proper k -partition R_1, \dots, R_k of its rows and C_1, \dots, C_k of its columns is

$$\text{disc}(\mathbf{A}; R_1, \dots, R_k, C_1, \dots, C_k) = \max_{1 \leq u, v \leq k} \max_{X \subset R_u, Y \subset C_v} \text{disc}(X, Y; R_u, C_v), \quad (7)$$

where

$$\begin{aligned} \text{disc}(X, Y; R_u, C_v) &= \frac{|a(X, Y) - \rho(R_u, C_v) \text{Vol}(X) \text{Vol}(Y)|}{\sqrt{\text{Vol}(X) \text{Vol}(Y)}} \\ &= |\rho(X, Y) - \rho(R_u, C_v)| \sqrt{\text{Vol}(X) \text{Vol}(Y)}. \end{aligned} \quad (8)$$

Here $a(X, Y) = \sum_{i \in X} \sum_{j \in Y} a_{ij}$ is the cut between $X \subset R_u$ and $Y \subset C_v$, $\text{Vol}(X) = \sum_{i \in X} d_{row,i}$ 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 \mathbf{A} is

$$\text{disc}_k(\mathbf{A}) = \min_{\substack{R_1, \dots, R_k \\ C_1, \dots, C_k}} \text{disc}(\mathbf{A}; R_1, \dots, R_k, C_1, \dots, C_k).$$

In [10], we proved that given the $m \times n$ rectangular array \mathbf{A} , the following spectral biclustering results in row-column cluster pairs of small discrepancy. The clusters R_1, \dots, R_k of the rows and C_1, \dots, 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 $(\mathbf{D}_{row}^{-1/2} \mathbf{v}_1, \dots, \mathbf{D}_{row}^{-1/2} \mathbf{v}_{k-1})$ and $(\mathbf{D}_{col}^{-1/2} \mathbf{u}_1, \dots, \mathbf{D}_{col}^{-1/2} \mathbf{u}_{k-1})$, respectively, where $\mathbf{v}_i, \mathbf{u}_i$ is the unit norm singular vector pair corresponding to s_i ($i = 1, \dots, k-1$). Recall that these partitions minimize the weighted k -variances $\tilde{S}_{k,row}^2$ and $\tilde{S}_{k,col}^2$ of these row- and column-representatives introduced in (4). Then, under some balancing conditions for the margins and for the cluster sizes, we proved that $\text{disc}_k(\mathbf{A}) = O(\sqrt{2k}(\tilde{S}_{k,row} + \tilde{S}_{k,col}) + s_k)$.

In the special case when $m = n$ and \mathbf{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 $G = (V, \mathbf{A}_n)$, where the singular values of $\mathbf{M}_{D,n}$ are the numbers $s_i = |\mu_i|$ ($i = 1, \dots, n$).

Proposition 4. Let $G = (V, \mathbf{W})$ be a connected edge-weighted graph on n vertices, with generalized degrees d_1, \dots, d_n and degree matrix \mathbf{D} . Assume that $\text{Vol}(V) = 1$, and there are no dominant vertices,

i.e., $d_i = \Theta(1/n)$, $i = 1, \dots, n$, as $n \rightarrow \infty$. Let the eigenvalues of $\mathbf{M}_{D,n}$, enumerated in decreasing absolute values, be

$$1 \geq |\mu_{1,n}| \geq \dots \geq |\mu_{k-1,n}| > \varepsilon \geq |\mu_{k,n}| \geq \dots \geq |\mu_{n,n}| = 0.$$

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

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

where $\rho(C_i) = \frac{w(V_i, V_i)}{\text{Vol}^2(V_i)}$ 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,*

$$s_k = \mathcal{O}(\sqrt{\log m \log n}) \text{disc}_k(\mathbf{A})$$

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

For the proof we need the following lemmas. Lemma 3 of Bollobás and Nikiforov [14] states that to 5 every $0 < \varepsilon < 1$ and vector $\mathbf{x} \in \mathbb{C}^n$, $\|\mathbf{x}\| = 1$, there exists a vector $\mathbf{y} \in \mathbb{C}^n$ such that its coordinates take no more than $\lceil \frac{8\pi}{\varepsilon} \rceil \lceil \frac{4}{\varepsilon} \log \frac{2n}{\varepsilon} \rceil$ distinct values and $\|\mathbf{x} - \mathbf{y}\| \leq \varepsilon$. Lemma 3 of Butler [18] can be traced back to this one. It states that to any vector $\mathbf{x} \in \mathbb{C}^n$, $\|\mathbf{x}\| = 1$ and diagonal matrix \mathbf{D} of positive real diagonal entries, one can construct a step-vector $\mathbf{y} \in \mathbb{C}^n$ such that $\|\mathbf{x} - \mathbf{D}\mathbf{y}\| \leq \frac{1}{3}$, $\|\mathbf{D}\mathbf{y}\| \leq 1$, and \mathbf{y} has at most $\Theta(\log n)$ distinct coordinates. We will also use the following lemma that we constructed just 10 for this purpose.

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

$$a'_{ab} := \frac{a(R_u, C_v)}{\sqrt{\text{VOL}(R_u) \text{VOL}(C_v)}}, \quad u = 1, \dots, k; v = 1, \dots, \ell,$$

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

$$|\langle \mathbf{x}, \mathbf{A}\mathbf{y} \rangle| \leq \|\mathbf{A}'\| \cdot \|\mathbf{D}_r^{1/2} \mathbf{x}\| \cdot \|\mathbf{D}_c^{1/2} \mathbf{y}\|,$$

where $\|\mathbf{A}'\|$ denotes the spectral norm, that is the largest singular value of the real matrix \mathbf{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 \mathbf{A} , and the volumes are usually not the ones defined in Section 2; this is why they are denoted by VOL instead of Vol. 15

Proof of Lemma 2. For the distinct coordinates of \mathbf{x} and \mathbf{y} we introduce

$$x_i := \frac{x'_a}{\sqrt{\text{VOL}(R_a)}} \quad \text{if } i \in R_a \quad \text{and} \quad y_j := \frac{y'_b}{\sqrt{\text{VOL}(C_b)}} \quad \text{if } j \in C_b$$

with x'_a and y'_b that are coordinates of $\mathbf{x}' \in \mathbb{C}^k$ and $\mathbf{y}' \in \mathbb{C}^l$. Obviously, $\|\mathbf{D}_r^{1/2} \mathbf{x}\| = \|\mathbf{x}'\|$ and $\|\mathbf{D}_c^{1/2} \mathbf{y}\| = \|\mathbf{y}'\|$. Then, using $\bar{}$ for the complex conjugation,

$$\begin{aligned} |\langle \mathbf{x}, \mathbf{A} \mathbf{y} \rangle| &= \left| \sum_{i=1}^m \sum_{j=1}^n x_i \bar{y}_j c_{ij} \right| = \left| \sum_{a=1}^k \sum_{b=1}^l \frac{x'_a}{\sqrt{\text{Vol}(R_a)}} \frac{\bar{y}'_b}{\sqrt{\text{Vol}(C_b)}} c(R_a, C_b) \right| \\ &= \left| \sum_{a=1}^k \sum_{b=1}^l x'_a \bar{y}'_b c'_{ab} \right| = |\langle \mathbf{x}', \mathbf{A}' \mathbf{y}' \rangle| \leq s_{\max}(\mathbf{A}') \cdot \|\mathbf{x}'\| \cdot \|\mathbf{y}'\| \\ &= \|\mathbf{A}'\| \cdot \|\mathbf{D}_r^{1/2} \mathbf{x}\| \cdot \|\mathbf{D}_c^{1/2} \mathbf{y}\| \end{aligned}$$

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

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

$$|c(X, Y) - \rho(R_a, C_b) \text{Vol}(X) \text{Vol}(Y)| \leq \alpha \sqrt{\text{Vol}(X) \text{Vol}(Y)}. \quad (9)$$

Introducing the $m \times n$ matrix

$$\mathbf{F} = \mathbf{A} - \mathbf{D}_{\text{row}} \mathbf{R} \mathbf{D}_{\text{col}}, \quad (10)$$

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

$$\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2} = \mathbf{D}_{\text{row}}^{-1/2} \mathbf{A} \mathbf{D}_{\text{col}}^{-1/2} - \mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2} = \mathbf{A}_D - \mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2}.$$

Since the rank of the matrix $\mathbf{D}_{\text{row}}^{1/2} \mathbf{R} \mathbf{D}_{\text{col}}^{1/2}$ 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 \mathbf{A}_D :

$$s_k \leq s_{\max}(\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) = \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\|,$$

5 where $\|\cdot\|$ denotes the spectral norm.

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

$$|\langle \mathbf{v}, (\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) \mathbf{u} \rangle| = \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\|.$$

In view of Butler [18], there are stepwise constant vectors $\mathbf{x} \in \mathbb{C}^m$ and $\mathbf{y} \in \mathbb{C}^n$ such that $\|\mathbf{v} - \mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq \frac{1}{3}$, $\|\mathbf{u} - \mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq \frac{1}{3}$, $\|\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}\| \leq 1$, and $\|\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}\| \leq 1$; further,

$$\|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\| \leq \frac{9}{2} \left| \langle (\mathbf{D}_{\text{row}}^{1/2} \mathbf{x}), (\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}) (\mathbf{D}_{\text{col}}^{1/2} \mathbf{y}) \rangle \right| = \frac{9}{2} |\langle \mathbf{x}, \mathbf{F} \mathbf{y} \rangle|.$$

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

$$s_k \leq \|\mathbf{D}_{\text{row}}^{-1/2} \mathbf{F} \mathbf{D}_{\text{col}}^{-1/2}\| \leq \frac{9}{2} |\langle \mathbf{x}, \mathbf{F} \mathbf{y} \rangle|.$$

With the preliminary argument, \mathbf{x} takes on at most $r_1 = \Theta(\log m)$, and \mathbf{y} takes on at most $r_2 = \Theta(\log n)$ distinct values, which define the proper partitions P_1, \dots, P_{r_1} of the rows and Q_1, \dots, Q_{r_2} of the columns. Let us consider the subdivision of them with respect to R_1, \dots, R_k and C_1, \dots, C_k . In this way, we obtain the proper partition P'_1, \dots, P'_{ℓ_1} of the rows and Q'_1, \dots, Q'_{ℓ_2} of the columns with at most $\ell_1 = kr_1$ and

10 $\ell_2 = kr_2$ parts.

Now, we apply Lemma 2 to the matrix \mathbf{F} and to the step-vectors \mathbf{x} and \mathbf{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 \mathbf{F}' are

$$f'_{uv} := \frac{f(P'_u, Q'_v)}{\sqrt{\text{Vol}(P'_u) \text{Vol}(Q'_v)}}$$

and

$$|\langle \mathbf{x}, \mathbf{F}\mathbf{y} \rangle| \leq \|\mathbf{F}'\| \cdot \|\mathbf{D}_{row}^{1/2} \mathbf{x}\| \cdot \|\mathbf{D}_{col}^{1/2} \mathbf{y}\| \leq \|\mathbf{F}'\|.$$

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

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

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

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

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* $G = (V, \mathbf{W})$ is a special case of that of a rectangular array 5 in that its edge-weight matrix $\mathbf{W} = (w_{ij})$ is quadratic, but asymmetric: $w_{ij} \geq 0$ is the weight of the $i \rightarrow j$ edge ($i \neq j$) and $w_{ii} = 0$ ($i = 1, \dots, n$). 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. 10

Based on the singular values

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

of the normalized (asymmetric) 34×34 edge-weight matrix \mathbf{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. 15
2. Belgium, France, Germany, Ireland, Italy, Netherlands, Portugal, Spain, Switzerland, United Kingdom.
3. Denmark, Finland, Iceland, Norway, Sweden.

The column-clusters (immigration trait clusters) were:

1. Australia, Austria, Belgium, France, Greece, Israel, Italy, Luxembourg, Poland, Portugal, Spain, 20
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 25 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. 30

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. 35

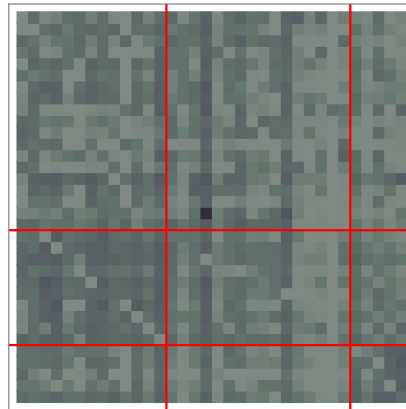


Fig. 4. Asymmetric adjacency matrix of the migration graph, where darker spots mean larger numbers while lighter spots mean smaller ones. Rows and columns are ordered according to the out- and in-cluster memberships, respectively; further, the clusters are separated by red lines.

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 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
 5 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.

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