Relating multiway discrepancy and singular values of contingency tables

Marianna Bolla

Institute of Mathematics, Budapest University of Technology and Economics
E-mail: marib@math.bme.hu

Abstract

The $k$-way discrepancy $\text{disc}_k(C)$ of a rectangular array $C$ of nonnegative entries is the minimum of the maxima of the within- and between-cluster discrepancies that can be obtained by simultaneous $k$-clusterings (proper partitions) of its rows and columns. In Theorem 1, irrespective of the size of $C$, we give the following estimate for the $k$th largest non-trivial singular value of the normalized table:

$$s_k \leq 9\text{disc}_k(C)(k + 2 - 9k \ln \text{disc}_k(C)),$$

provided $\text{disc}_k(C) < 1$ and $k \leq \text{rank}(C)$. This statement is the converse of Theorem 7 of Bolla [6], and the proof uses some lemmas and ideas of Butler [9], where only the $k=1$ case is treated, in which case our upper bound is the tighter. The result naturally extends to the singular values of the normalized adjacency matrix of a weighted undirected or directed graph, and it gives some spectral characterization of generalized random or quasirandom graphs.

Keywords: multiway discrepancy; singular values; normalized table; weighted graphs; directed graphs; generalized random graphs.

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1 Introduction

In many applications, for example when microarrays are analyzed, our data are collected in the form of an $m \times n$ rectangular array $C = (c_{ij})$ of nonnegative real entries, called contingency table. We assume that $C$ is non-decomposable, i.e., $CC^T$ (when $m \leq n$) or $C^TC$ (when $m > n$) is irreducible. Consequently, the row-sums $d_{\text{row},i} = \sum_{j=1}^n c_{ij}$ and column-sums $d_{\text{col},j} = \sum_{i=1}^m c_{ij}$ of $C$ are strictly positive, and the diagonal matrices $D_{\text{row}} = \text{diag}(d_{\text{row},1}, \ldots, d_{\text{row},m})$ and $D_{\text{col}} = \text{diag}(d_{\text{col},1}, \ldots, d_{\text{col},n})$ are regular. Without loss of generality, we also assume that $\sum_{i=1}^n \sum_{j=1}^m c_{ij} = 1$, since neither our main object, the normalized table

$$C_{\text{nor}} = D_{\text{row}}^{-1/2}CD_{\text{row}}^{-1/2},$$

nor the multiway discrepancies to be introduced are affected by the scaling of the entries of $C$. It is well known (see e.g., [4]) that the singular values of $C_{\text{nor}}$ are in the [0,1] interval. Enumerated in non-increasing order, they are the real numbers

$$1 = s_0 > s_1 \geq \cdots \geq s_{r-1} > s_r = \cdots = s_{n-1} = 0,$$

where $r = \text{rank}(C)$. When $C$ is non-decomposable, 1 is a single singular value, and it is denoted by $s_0$, since it belongs to the trivial singular vector pair, which will be disregarded in some further calculations.

Our purpose is to find relations between the $k$th nontrivial singular value $s_k$ of $C_{\text{nor}}$ and the minimum $k$-way discrepancy of $C$ defined herein.
Definition 1 The $k$-way discrepancy of the contingency table $C$ in the proper $k$-partition $R_1, \ldots, R_k$ of its rows and $C_1, \ldots, C_k$ of its columns is

$$
\text{disc}_{R_1, \ldots, R_k}(C) = \max_{1 \leq a < b \leq k} \frac{|c(X, Y) - \rho(R_a, C_b)\text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}},
$$

(2)

where $c(X, Y) = \sum_{i \in X} \sum_{j \in Y} c_{ij}$ is the cut between $X \subset R_a$ and $Y \subset C_b$, $\text{Vol}(X) = \sum_{i \in X} d_{\text{row}, i}$ is the volume of the row-subset $X$, $\text{Vol}(Y) = \sum_{j \in Y} d_{\text{col}, j}$ is the volume of the column-subset $Y$, whereas $\rho(R_a, C_b) = \frac{c(R_a, C_b)}{\sqrt{\text{Vol}(R_a)\text{Vol}(C_b)}}$ denotes the relative density between $R_a$ and $C_b$. The $k$-way discrepancy of $C$ itself is

$$
\text{disc}_k(C) = \min_{R_1, \ldots, R_k} \text{disc}_{R_1, \ldots, R_k}(C).
$$

These notions naturally extend to edge-weighted graphs. A weighted undirected graph $G = (V, W)$ is uniquely characterized by its weighted adjacency matrix $W$, which is a symmetric contingency table of zero diagonal. With the diagonal degree matrix $D$, the normalized adjacency matrix is $W_{\text{nor}} = D^{-1/2}WD^{-1/2}$, the singular values of which are the absolute values of its real eigenvalues. Definition 1 extends to this case as follows.

Definition 2 The $k$-way discrepancy of the undirected weighted graph $G = (V, W)$ in the proper $k$-partition $V_1, \ldots, V_k$ of its vertices is

$$
\text{disc}_{V_1, \ldots, V_k}(G) = \max_{1 \leq a < b \leq k} \frac{|w(X, Y) - \rho(V_a, V_b)\text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}}.
$$

The $k$-way discrepancy of the undirected weighted graph $G = (V, W)$ is

$$
\text{disc}_k(G) = \min_{V_1, \ldots, V_k} \text{disc}_{V_1, \ldots, V_k}(G).
$$

A directed weighted graph $G = (V, W)$ is described by its quadratic, but usually not symmetric weight matrix $W = (w_{ij})$ of zero diagonal, where $w_{ij}$ is the nonnegative weight of the $i \rightarrow j$ edge ($i \neq j$). With the diagonal in- and out-degree matrices, the normalized adjacency matrix is $W_{\text{nor}} = D_{\text{out}}^{-1/2}WD_{\text{in}}^{-1/2}$, the singular values of which enter into the estimation. Now Definition 1 can be formulated as follows.

Definition 3 The $k$-way discrepancy of the directed weighted graph $G = (V, W)$ in the in-clustering $V_{in,1}, \ldots, V_{in,k}$ and out-clustering $V_{out,1}, \ldots, V_{out,k}$ of its vertices is

$$
\text{disc}_{V_{in,1}, \ldots, V_{in,k}, V_{out,1}, \ldots, V_{out,k}}(G) = \max_{1 \leq a < b \leq k} \frac{|w(X, Y) - \rho(V_{out.a}, V_{in.b})\text{Vol}(X)\text{Vol}(Y)|}{\sqrt{\text{Vol}(X)\text{Vol}(Y)}}.
$$

The $k$-way discrepancy of the directed weighted graph $G = (V, W)$ is

$$
\text{disc}_k(G) = \min_{V_{in,1}, \ldots, V_{in,k}, V_{out,1}, \ldots, V_{out,k}} \text{disc}_{V_{in,1}, \ldots, V_{in,k}, V_{out,1}, \ldots, V_{out,k}}(G).
$$
The notion of discrepancy together with the Expander Mixing Lemma was first used for simple (sometimes regular) graphs, see e.g., Alon, Spencer, Hoory, Linial, Widgerson [1, 12], and extended to Hermitian matrices in Bollobás, Nikiforov [7]. In Chung, Graham, Wilson [10], the authors use the term quasi-rand-0 for simple graphs that satisfy any of some equivalent properties, some of them closely related to discrepancy and eigenvalue separation. Chung and Graham [11] prove that ‘small’ discrepancy disc(G) = disc₁(G) causes eigenvalue ‘separation’; s₁ is ‘small’, i.e., separated from the trivial singular value 1, which is the edge of the spectrum. More exactly, they prove disc(G) ≤ s₁ (Expander Mixing Lemma for simple graphs), and also prove that for dense enough graphs some converse of this relation is true. At the same time, for sparse graphs, Bollobás and Nikiforov [7] describe a general construction when the converse implication is not true. Bilu and Linial [3] prove the converse of the Expander Mixing Lemma for simple regular graphs. Note that in Alon et al. [2], the authors relax the notion of eigenvalue separation to essential eigenvalue separation (by introducing a parameter for it and requiring the separation only for the eigenvalues of a relatively large part of the graph). Then they prove bilateral relations between the constants of this kind of eigenvalue separation and discrepancy.

For a general contingency table C, Butler [9] proves the following forward and backward statement in the k = 1 case: the largest non-trivial singular value, s₁, of C_{nor} is estimated from above and from below with the overall discrepancy disc(C) = disc₁(C) of the table as

\[ \text{disc}(C) \leq s_1 \leq 150\text{disc}(C)(1 - 8 \ln \text{disc}(C)). \]  

Since s₁ < 1, the upper estimate makes sense for very small discrepancy, in particular, for disc(C) ≤ 8.868 × 10⁻⁵ and spectral gap larger than 1 − 8.868 × 10⁻⁵.

But what if the gap is not at the end of the spectrum? Now, more generally, we want to find similar relations between discₖ(C) and sₖ if 1 < k ≤ rank(C) is an integer. In the forward direction, in Bolla [6], we managed to prove the following. Given the m × n contingency table C, consider the spectral clusters R₁, . . . , Rₖ of its rows and C₁, . . . , Cₖ of its columns, obtained by applying the k-means algorithm for the (k − 1)-dimensional row- and column representatives, defined as the row vectors of the matrices of column vectors (D₋₁/²ᵣᵢv₁, . . . , D₋₁/²ᵣᵢvk−₁) and (D₋₁/²ᶜᵢᵤ₁, . . . , D₋₁/²ᶜᵢᵤk−₁), respectively, where vᵢ, uᵢ is the unit norm singular vector pair corresponding to sᵢ (i = 1, . . . , k − 1). In fact, these partitions minimize the weighted k-variances σᵢ² and σⱼ² of these row- and column-representatives. Then, under some balancing conditions for dᵣᵢ’s and dᶜᵢ’s (there are no dominant rows and columns) and for the cluster sizes, we proved that disc′ₖ(C) = O(√2k(σᵢ + σⱼ) + sₖ). Here disc′ₖ(C) is a somewhat modified version of the k-way discrepancy, introduced after the notion of volume-regular pairs of Alon et al. [2]; the only difference is that in the definition of disc′ₖ(C) we substitute √Vol(Rₖ)Vol(Cₖ) for √Vol(X)Vol(Y) into the denominator of Formula (2). In accordance with the original definition of the discrepancy in Szemerédi’s Regularity Lemma [15] for simple graphs, in (2), we may take the maximum over subsets X ⊂ Vₖ, Y ⊂ Vₖ such that Vol(X) ≥ εVol(Vₖ) and Vol(Y) ≥ εVol(Vₖ) with some fixed ε > 0. If we impose similar conditions on the row- and column-subsets, our result also implies that
disc_k(C) is of order \(\sqrt{2k}(\sigma_r + \sigma_c) + s_k\).

In Section 2, we will prove the backward statement, namely, we give an upper bound for \(s_k\) by means of the \(k\)-way discrepancy of Definition 1.

**Theorem 1** For every non-decomposable contingency table \(C\) and integer \(1 \leq k \leq \text{rank}(C)\),

\[
s_k \leq 9 \text{disc}_k(C)(k + 2 - 9k \ln \text{disc}_k(C))\]

provided \(\text{disc}_k(C) < 1\), where \(s_k\) is the \(k\)th largest non-trivial singular value of the normalized table \(C_{nor}\) introduced in (1).

Note that \(\text{disc}_k(C) < 1\) is not a peculiar requirement, since in view of \(s_k < 1\), the upper bound of the theorem has relevance only for \(\text{disc}_k(C)\) much smaller than 1; for example, for \(\text{disc}_1(C) \leq 1.866 \times 10^{-3}\), \(\text{disc}_2(C) \leq 8.459 \times 10^{-4}\), \(\text{disc}_3(C) \leq 5.329 \times 10^{-4}\), etc.

The message of this theorem is that the \(k\)-way discrepancy, when it is 'small' enough, suppresses \(s_k\). From the forward statement we know, that \(s_k\) together with 'small' enough \(\sigma_r\) and \(\sigma_c\) also suppresses the \(k\)-way discrepancy. Using perturbation theory of spectral subspaces, in [5] (in the framework of weighted graphs), we also discuss that a 'large' gap between \(s_{k-1}\) and \(s_k\) suppresses \(\sigma_r\) and \(\sigma_c\). Therefore, if we want to find row–column cluster pairs of small discrepancy, we must select a \(k\) such that there is a remarkable gap between \(s_{k-1}\) and \(s_k\); further \(s_k\) is small enough. Moreover, by using this \(k\) and the construction in the proof of the forward statement of [6], we are able to find these clusters with spectral clustering tools. It makes sense, for example, when we want to find clusters of genes and conditions simultaneously in microarrays so that genes of the same row-cluster would 'equally' influence conditions of the same column-cluster. These issues together with other trails and dead-ends of the proof, which yield weaker estimates though may be instructive, are to be discussed in Section 3.

The above considerations are applicable to unweighted or weighted, undirected or directed graphs as special cases. For simple graphs, our result means that the absolute values of the eigenvalues of the normalized adjacency matrix should be considered. In this case, the clusters or cluster-pairs of small discrepancy behave like expanders or bipartite expanders. In another context, they resemble the generalized random or quasirandom graphs of Lovász, Sós, Simonovits [13, 14]. Our statements indicate that the number of the clusters, and the clusters themselves of these structures can be concluded via their normalized spectra and spectral clustering tools.

### 2 Proof of Theorem 1

Assume that \(\alpha := \text{disc}_k(C) < 1\) and it 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 \(C\); i.e., for every \(R_a, C_b\) pair and \(X \subset R_a, Y \subset C_b\) we have

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

(4)

Our purpose is to put Inequality (4) in matrix form by using indicator vectors and introducing the \(m \times n\) auxiliary matrix

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

(5)
where \( \mathbf{R} = (\rho(R_a, C_b)) \) is the \( m \times n \) block-matrix of \( k \times k \) blocks with entries equal to \( \rho(R_a, C_b) \) over the block \( R_a \times C_b \). With the indicator vectors \( \mathbf{1}_X \) and \( \mathbf{1}_Y \) of \( X \subset R_a \) and \( Y \subset C_b \), Inequality (4) has the following equivalent form:

\[
\langle \mathbf{1}_X, \mathbf{F}_Y \rangle \leq \alpha \sqrt{\langle \mathbf{1}_X, \mathbf{C}_1 \rangle \langle \mathbf{1}_m, \mathbf{C}_1 \rangle}
\]  

(6)

where \( \mathbf{1}_n \) denotes the all 1’s vector of size \( n \) and \( \langle \ldots \rangle \) denotes the (possibly complex) inner product. Note that in the possession of real (column) vectors and matrices, \( \langle \ldots \rangle \) can be written in terms of matrix-vector multiplications with transpositions; for example, \( \langle \mathbf{1}_X, \mathbf{F}_Y \rangle = \mathbf{1}_X^T \mathbf{F}_Y \). At the same time, Equation (5) yields

\[
\mathbf{D}_{row}^{-1/2} \mathbf{F} \mathbf{D}_{col}^{-1/2} = \mathbf{D}_{row}^{-1/2} \mathbf{C} \mathbf{D}_{col}^{-1/2} - \mathbf{D}_{row}^{1/2} \mathbf{R} \mathbf{D}_{col}^{1/2} = \mathbf{C}_{nor} - \mathbf{D}_{row}^{1/2} \mathbf{R} \mathbf{D}_{col}^{1/2}.
\]

Since the rank of the matrix \( \mathbf{D}_{row}^{1/2} \mathbf{R} \mathbf{D}_{col}^{1/2} \) is at most \( k \), by Theorem 3 of Thompson\(^1\) [16], 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 \( \mathbf{C}_{nor} \):

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

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 \( \mathbf{D}_{row}^{-1/2} \mathbf{F} \mathbf{D}_{col}^{-1/2} \), i.e.,

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

In view of Lemma 3 of Butler [9], there are stepwise constant vectors \( \mathbf{x} \in \mathbb{C}^m \) and \( \mathbf{y} \in \mathbb{C}^n \) such that \( \| \mathbf{v} - \mathbf{D}_{row}^{-1/2} \mathbf{x} \| \leq \frac{1}{5} \) and \( \| \mathbf{u} - \mathbf{D}_{col}^{-1/2} \mathbf{y} \| \leq \frac{1}{5} \); further, \( \| \mathbf{D}_{row}^{-1/2} \mathbf{x} \| \leq 1 \) and \( \| \mathbf{D}_{col}^{-1/2} \mathbf{y} \| \leq 1 \). Then Lemma 4 of Butler [9] yields

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

Now we will use the construction in the proof of the Lemma 3 [9] in the special case when the vectors \( \mathbf{v} = (v_s)_{s=1}^m \) and \( \mathbf{u} = (u_s)_{s=1}^n \), to be approximated, have real coordinates. Therefore, only the following three types of coordinates of the approximating complex vectors \( \mathbf{x} = (x_s)_{s=1}^m \) and \( \mathbf{y} = (y_s)_{s=1}^n \) will appear. If \( v_s = 0 \), then \( x_s = 0 \) too; if \( v_s > 0 \), then \( x_s = \left( \frac{4}{5} \right)^j \) with some integer \( j \); if \( v_s < 0 \), then \( x_s = \left( \frac{4}{5} \right)^j e^{\frac{2\pi}{5} j} \) with some integer \( j \). Likewise, if \( u_s = 0 \), then \( y_s = 0 \) too; if \( u_s > 0 \), then \( y_s = \left( \frac{4}{5} \right)^{\ell} \) with some integer \( \ell \); if \( u_s < 0 \), then \( y_s = \left( \frac{4}{5} \right)^{\ell} e^{\frac{2\pi}{5} j} \) with some integer \( \ell \). With these observations, the step-vectors \( \mathbf{x} \) and \( \mathbf{y} \) can be written as the following finite sums with respect to the integers \( j \) and \( \ell \):

\[
\mathbf{x} = \sum_j \left( \frac{4}{5} \right)^j \mathbf{x}^{(j)}, \quad \mathbf{x}^{(j)} = \sum_{a=1}^k (1 \mathbf{x}_{ja} + e^{\frac{2\pi}{5} j} \mathbf{x}_{ja}),
\]

where

\(^1\)Actually, Thompson stated the theorem for square matrices, but in the possession of a rectangular one, we can supplement it with zero rows or columns to make it quadratic; further, the nonzero singular values of the so obtained square matrix are the same as those of the rectangular, supplemented with additional zero singular values that will not alter the shifted interlacing facts.
\( X_{ja1} = \{ s : x_s = \left( \frac{4}{5} \right)^j, s \in R_a \} \) and \( X_{ja2} = \{ s : x_s = \left( \frac{4}{5} \right)^j e^{\frac{2\pi}{3}i}, s \in R_a \} \); likewise,

\[
y = \sum_i \left( \frac{4}{5} \right)^i y^{(i)}, \quad y^{(i)} = \sum_{b=1}^{k} (1_{\mathcal{Y}_{b1}} + e^{\frac{2\pi}{3}i} 1_{\mathcal{Y}_{b2}}),
\]

where

\[
\mathcal{Y}_{b1} = \{ s : y_s = \left( \frac{4}{5} \right)^i, s \in C_b \} \quad \text{and} \quad \mathcal{Y}_{b2} = \{ s : y_s = \left( \frac{4}{5} \right)^i e^{\frac{2\pi}{3}i}, s \in C_b \}.
\]

Then

\[
|\langle x^{(j)}, F_y^{(i)} \rangle| \leq \sum_{ab} \sum_{pq} \sum_{k} \sum_{2} |1_{\mathcal{X}_{jap}}, F_{1}\mathcal{Y}_{bq}| \leq \sum_{a1} \sum_{b1} \sum_{p1} \sum_{q1} \alpha \sqrt{|1_{\mathcal{X}_{jap}}, C1n|1m, C11_{\mathcal{Y}_{bq}}|}
\]

\[
\leq \alpha2k \sqrt{\sum_{a1} \sum_{b1} \sum_{p1} \sum_{q1} \sum_{k} \sum_{2} |1_{\mathcal{X}_{jap}}, C1n|1m, C11_{\mathcal{Y}_{bq}}|}
\]

\[
= 2k\alpha \sqrt{|\langle x^{(j)}, C1n |1m, C|y^{(i)} \rangle|},
\]

where in the first inequality we used that \(|e^{\frac{2\pi}{3}i}| = 1\), in the second one we used (6), while in the last one, the Cauchy–Schwarz inequality with \(4k^2\) terms. We also introduced the notation \(|z| = |(z_n)|_{n=1}^n\) for the real vector, the coordinates of which are the absolute values of the corresponding coordinates of the (possibly complex) vector \(z\). In the same spirit, let \(|\mathbf{M}|\) denote the matrix whose entries are the absolute values of the corresponding entries of \(\mathbf{M}\) (we will use this only for real matrices). With this formalism, this is the right moment to prove the following inequalities that will be used soon to finish the proof:

\[
\sum_{i} |\langle x^{(j)}, F_y^{(i)} \rangle| \leq 2|\langle x^{(j)}, C1n \rangle|, \quad \sum_{j} |\langle x^{(j)}, F_y^{(i)} \rangle| \leq 2|1m, C|y^{(i)} |\rangle. \quad (8)
\]

Since the two inequalities are of the same flavor, it suffices to prove only the first one. Note that it is here, where we use the exact definition of \(F\) as follows.

\[
\sum_{i} |\langle x^{(j)}, F_y^{(i)} \rangle| \leq |\langle x^{(j)}, |F| \sum_{i} y^{(i)} \rangle| \leq |\langle x^{(j)}, (C + D_{row} \mathbf{RD}_{col})1_n \rangle| = 2|\langle x^{(j)}, C1n \rangle|
\]

because \(|y^{(i)}|\) is a 0-1 vector and \(C + D_{row} \mathbf{RD}_{col}\) is a (real) matrix of nonnegative entries. We also used that the \(i\)th coordinate of the vector \((C + D_{row} \mathbf{RD}_{col})1_n\) for \(i \in R_a\) is

\[
d_{row,i} \left( 1 + \sum_{b=1}^{k} \rho(R_a, C_b) \text{Vol}(C_b) \right) = 2d_{row,i}
\]
(here we utilized that the sum of the entries of \( C \) is 1), and therefore,

\[
(C + D_{row}RD_{col})1_n = 2C1_n.
\]

Finally, we will finish the proof with similar calculations as in [9]. Let us further estimate

\[
\langle x, Fy \rangle = \sum_j \sum_{\ell} \left( \frac{4}{5} \right) j^\ell \left( \langle x^{(j)}, F \rangle \right) \left( \frac{4}{5} \right) y^{(\ell)}.
\]

Put \( \gamma := \log_{4/5} \alpha \); in view of \( \alpha < 1, \gamma > 0 \) holds. Then we divide the above summation into three parts as follows.

\[
|\langle x, Fy \rangle| \leq \sum_j \sum_{\ell} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle|
\]

\[
= \sum_{|j-\ell| \leq \gamma} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle| + \sum_{j-\ell > \gamma} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle| + \sum_{j-\ell < -\gamma} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle|.
\]

The three terms are estimated separately. Term (a) can be bounded from above as follows:

\[
\sum_{|j-\ell| \leq \gamma} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle| \leq 2k\alpha \sum_{|j-\ell| \leq \gamma} \sqrt{\left( \frac{4}{5} \right)^{2j} |\langle x^{(j)}, C1_n \rangle| \left( \frac{4}{5} \right)^{2\ell} |\langle 1_m, C|y^{(\ell)} \rangle|}
\]

\[
\leq \left( * \right) k\alpha \sum_{|j-\ell| \leq \gamma} \left[ \left( \frac{4}{5} \right)^{2j} |\langle x^{(j)}, C1_n \rangle| + \left( \frac{4}{5} \right)^{2\ell} |\langle 1_m, C|y^{(\ell)} \rangle| \right]
\]

\[
\leq \left( ** \right) k\alpha(2\gamma + 1) \left[ \sum_j \left( \frac{4}{5} \right)^{2j} |\langle x^{(j)}, C1_n \rangle| + \sum_{\ell} \left( \frac{4}{5} \right)^{2\ell} |\langle 1_m, C|y^{(\ell)} \rangle| \right],
\]

\[
\leq \left( *** \right) 2k\alpha(2\gamma + 1),
\]

where in the first inequality, the estimate of (7) and in (*), the geometric-arithmetic mean inequality were used; (***) comes from the fact that in summation (a), for fixed \( j \) or \( \ell \), any term can show up at most \( 2\gamma + 1 \) times, and (****) is due to the easy observation that

\[
\sum_j \left( \frac{4}{5} \right)^{2j} |\langle x^{(j)}, C1_n \rangle| = \|D_{row}^{1/2}x\|^2 \leq 1,
\]

\[
\sum_{\ell} \left( \frac{4}{5} \right)^{2\ell} |\langle 1_m, C|y^{(\ell)} \rangle| = \|D_{col}^{1/2}y\|^2 \leq 1.
\]

\[
\sum_j \left( \frac{4}{5} \right)^{2j} |\langle x^{(j)}, C1_n \rangle| = \|D_{row}^{1/2}x\|^2 \leq 1,
\]

Terms (b) and (c) are of similar appearance (the role of \( j \) and \( \ell \) is symmetric in them), therefore, we will estimate only (b). Here \( j-\ell > \gamma \), yielding \( j+\ell > 2\ell+\gamma \).

Therefore,

\[
\sum_{j-\ell > \gamma} \left( \frac{4}{5} \right) j^\ell |\langle x^{(j)}, Fy^{(\ell)} \rangle| \leq \sum_{\ell} \left( \frac{4}{5} \right)^{2\ell} \sum_j |\langle x^{(j)}, Fy^{(\ell)} \rangle|
\]

\[
\leq \left( ** \right) \sum_{\ell} \left( \frac{4}{5} \right)^{2\ell} \sum_j |\langle x^{(j)}, Fy^{(\ell)} \rangle|
\]

\[
= 2\left( \frac{4}{5} \right)^\gamma \sum_{\ell} \left( \frac{4}{5} \right)^{2\ell} |\langle 1_m, C|y^{(\ell)} \rangle| \leq 2\left( \frac{4}{5} \right)^\gamma.
\]
where, in the second and third inequalities, (8) and (9) were used. Consequently, (c) can also be estimated from above with $2(\frac{4}{5})^\gamma$.

Collecting the so obtained estimates together, we get

$$s_k \leq \frac{9}{2} |\langle x, Fy \rangle| \leq \frac{9}{2} \left[ 2k\alpha(2\gamma + 1) + 4(\frac{4}{5})^\gamma \right] = 9\alpha \left[ 2\frac{k\ln\alpha}{\ln\frac{4}{5}} + k + 2 \right] \leq 9\alpha[2k(-4.5) \ln\alpha + k + 2] = 9\alpha(k + 2 - 9k\ln\alpha),$$

that was to be proved$^2$.

3 Some weaker results and conclusions

Now about our first attempts to prove something like Theorem 1, because they may be informative for the reader.

- First we wanted to use Lemma 3 of Bollobás and Nikiforov [7], since, in addition, it specifies the number of distinct coordinates of the approximating step-vector. This lemma states that to every $0 < \varepsilon < 1$ and vector $x \in \mathbb{C}^n$, with $\|x\| = 1$, there is a vector $y \in \mathbb{C}^n$ such that its coordinates take no more than

$$\left\lfloor \frac{8\pi}{\varepsilon} \right\rfloor \left\lfloor \frac{4}{\varepsilon} \log \frac{2n}{\varepsilon} \right\rfloor \tag{10}$$

values and $\|x - y\| \leq \varepsilon$.

Note that this lemma implies Lemma 3 of Butler [9], which states that to any unit-norm vector $x \in \mathbb{C}^n$ and diagonal matrix $D$ of positive diagonal entries, one can construct a step-vector $y \in \mathbb{C}^n$ such that $\|x - Dy\| \leq \varepsilon$ and $\|Dy\| \leq 1$. Even the construction of the two lemmas are similar.

In our case, $x \in \mathbb{R}^n$ and we need $1/3$ precision. Given the diagonal matrix $D$ of positive diagonal entries, we will now construct a step-vector $y$ of complex entries such that $\|x - Dy\| \leq 1/3$, by merely using Lemma 3 of [7]. First set $f := \|D^{-1}x\|$ and $d := \|D\| = \max_i d_i$. Then, by [7], to the unit-norm vector $D^{-1}x/f$ and to $0 < \varepsilon < 1$ there is a step-vector $y \in \mathbb{C}^n$, with the same number of different coordinates as in (10), such that

$$\left\| \frac{D^{-1}x}{f} - y \right\| \leq \varepsilon.$$

The step-vector $z = fy \in \mathbb{C}^n$, with the same number of different coordinates as in $y$, will do for us, since with an appropriate $\varepsilon$ we can reach that $\|x - Dz\| \leq \frac{1}{3}$. Indeed,

$$\varepsilon \geq \left\| \frac{D^{-1}x}{f} - z \right\| = \frac{1}{f} \|D^{-1}(x-Dz)\| \geq \frac{1}{f} \min_i \frac{1}{d_i} \|x-Dz\| = \frac{1}{f} \|x-Dz\|.$$

$^2$For $k = 1$, our upper bound is tighter than that of (3); hence, outperforms the result of Theorem 2 of [9]. The difference comes from the fact that the coordinates of the singular vectors of a real matrix are real numbers; therefore, the step-vectors, constructed in the proof, can have complex coordinates only with argument $\pm \frac{2\pi}{28}$. Though, Butler also starts with a real matrix, he takes into account all the arguments $\pm \frac{2\pi}{28} \ell$ ($\ell = 0, 1, \ldots, 28$), whereas, in our proof, only the $\ell = 0$ and $\ell = 14$ cases are considered (the first one yielding real, while the second one an indeed complex coordinate with the aforementioned argument). This is where our gain comes from.
Therefore,
\[ \|x - Dz\| \leq fd\varepsilon = \frac{1}{3} \]
holds with \( \varepsilon = \frac{1}{\sqrt{3}} \) that cannot exceed \( \frac{1}{3} \), since \( fd \geq 1 \). This can be seen from the following argument:

\[ 1 = \|x\| = \|DD^{-1}x\| \leq \|D\| \cdot \|D^{-1}x\| = df. \]

Eventually, by the construction of [7], \( |y_j| \leq \frac{|x_j|}{d_j} \), \( j = 1, \ldots, n \). Therefore,
\[ |z_j| = f|y_j| \leq \frac{|x_j|}{d_j}, \quad \text{and} \quad |d_jz_j| \leq |x_j|, \quad \forall j. \]
Consequently, \( \|Dz\| \leq \|x\| = 1 \).

The main implication of this fact is that the maximal number of distinct coordinates of the step-vector in Lemma 3 of [9] is also of order \( \log n \), and we wanted to make use of this fact in the first attempts of the proof of some backward statement. For this purpose, we managed to prove the following lemma, inspired by Lemma 4 of [7], though, in a more general setup. We will give the proof too, since it may be of interest for its own right.

**Lemma 1** Let \( \mathbf{C} \) be an \( m \times n \) matrix of nonnegative 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 \( \mathbf{C} \)), 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 \( R_1, \ldots, R_k \) and \( C_1, \ldots, C_\ell \) 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 \( C_1, \ldots, C_\ell \), respectively. The \( k \times \ell \) real matrix \( \mathbf{C}' = (c'_{ab}) \) is defined by

\[ c'_{ab} := \frac{c(R_a, C_b)}{\sqrt{\text{VOL}(R_a)\text{VOL}(C_b)}}, \quad a = 1, \ldots, k; \ b = 1, \ldots, \ell, \]

where \( c(R_a, C_b) \) is the usual cut of \( \mathbf{C} \) between \( R_a \) and \( C_b \), whereas \( \text{VOL}(R_a) = \sum_{i \in R_a} d_{r,i} \) and \( \text{VOL}(C_b) = \sum_{j \in C_b} d_{c,j} \). Then

\[ |\langle x, Cy \rangle| \leq \|\mathbf{C}'\| \cdot \|\mathbf{D}_r^{1/2}x\| \cdot \|\mathbf{D}_c^{1/2}y\|, \]

where \( \|\mathbf{C}'\| \) denotes the spectral norm, that is the largest singular value of the real matrix \( \mathbf{C}' \), 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 \( \mathbf{C} \), and the volumes are usually not the ones defined in Section 1; this is why they are denoted by \( \text{VOL} \) instead of \( \text{Vol} \).

**Proof of Lemma 1** For the distinct coordinates of \( x \) and \( y \) we introduce

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

with \( x'_a \) and \( y'_b \) that are coordinates of \( x' \in \mathbb{C}^k \) and \( y' \in \mathbb{C}^\ell \). Obviously, \( \|\mathbf{D}_r^{1/2}x\| = \|x'\| \) and \( \|\mathbf{D}_c^{1/2}y\| = \|y'\| \). Then, using - for the complex
Another dead-end was the attempt with the following matrix $F$ of $E$:

$$
\langle x, Cy \rangle = \left| \sum_{i=1}^{m} \sum_{j=1}^{n} x_i y_j c_{ij} \right| = \left| \sum_{a=1}^{k} \sum_{b=1}^{l} \frac{x_a'}{\sqrt{\text{VOL}(R_a)}} \frac{y_b'}{\sqrt{\text{VOL}(C_b)}} c(R_a, C_b) \right|
$$

$$
= \left| \sum_{a=1}^{k} \sum_{b=1}^{l} x_a' y_b' c_{ab}' \right| = \langle x', C'y' \rangle \leq s_{max}(C') \cdot \|x'\| \cdot \|y'\|
$$

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

Using this lemma and the starting steps of the proof of Theorem 1, with the matrix $F$ defined in (5) and the constructed step-vectors $x \in C^m$, $y \in C^n$, we have

$$s_k \leq \|D_{row}^{-1/2}FD_{col}^{-1/2} \| \leq \frac{9}{2}\|x, Fy\|.
$$

We also know from [7] and the preliminary argument that $x$ 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 $\ell_1 = kr_1$ and $\ell_2 = kr_2$ parts.

Now, we apply Lemma 1 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 $d_{row,i}$’s and $d_{col,j}$’s, respectively. In view of the lemma, the entries of the $\ell_1 \times \ell_2$ matrix $F'$ are

$$f_{ab}' := \frac{f(P_a', Q_b')}{\sqrt{\text{Vol}(P_a')} \sqrt{\text{Vol}(Q_b')}}$$

and

$$\|x, Fy\| \leq \|F'\| \cdot \|D_{row}^{1/2}x\| \cdot \|D_{col}^{1/2}y\| \leq \|F'\|.
$$

But by a well-known linear algebra fact,

$$\|F'\| = s_{max}(F') \leq \sqrt{\ell_1 \ell_2} \max_{a \in \{1, \ldots, \ell_1\}} \max_{b \in \{1, \ldots, \ell_2\}} |f_{ab}'| \leq \ell \cdot \text{disc}_{R_1, \ldots, R_k}(C),$$

where $\ell = \sqrt{\ell_1 \ell_2}$ and we used Formula (2) for the discrepancy. Consequently,

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

follows. The drawback is that the upper bound contains $\ell = k \sqrt{r_1 r_2}$ which is of order $\sqrt{\log m \log n}$. Therefore, we prefer the estimate of Theorem 1 that does not contain the sizes of $C$.

- Another dead-end was the attempt with the following matrix $E$ instead of $F$ of (5):

$$E = C - D_{row} \hat{C} D_{col},$$

(11)
Finally, note that (see Theorem 1) do not depend on the size of the graph, there is a hope to given 
Borgs et al. [8]. Since the singular values of a compact operator tend to the 
lar value of the compact operator assigned to the limiting graphon, see 
largest non-trivial singular value of 
k > integer 
In the symmetric scenario [5], we considered a convergent sequence of 
variate statistics, namely, in correspondence analysis (see [4] for details).

tional expectation between the margins of 
C 
that the 
k spectral evidence of the Regularity Lemma [15].

The vectors ˆv_i and ˆu_i themselves were constructed via several SVDs in the 
proof of the forward statement of [6] so that D_{row}^{1/2} ˆv_i and D_{col}^{1/2} ˆu_i be ‘close’ to 
v_i and u_i, respectively, for i = 1, . . . , k − 1 (for i = 0, they coincide), where v_i ∈ R^m, u_i ∈ R^n is the unit-norm singular vector pair corresponding to s_i (i = 1, . . . , r). In particular, v_0 = (√d_{row,1}, . . . , √d_{row,m})^T 
and u_0 = (√d_{col,1}, . . . , √d_{col,n})^T.

The point is that the so-called error matrix E is close to the matrix 
D_{row}^{1/2}(C_{nor} - Σ_i=0^{k-1} s_i v_i u_i^T)D_{col}^{1/2}, and ∥C_{nor} - Σ_i=0^{k-1} s_i v_i u_i^T∥ = s_k. If 
now x ∈ C^n and y ∈ C^n are step-vectors such that ∥D_{row}^{1/2}x∥ ≤ 1, 
∥v_k - D_{row}^{1/2}x∥ ≤ 1/2 and ∥D_{col}^{1/2}y∥ ≤ 1, ∥u_k - D_{col}^{1/2}y∥ ≤ 1/2, then,

s_k ≤ 9/(2)∥(D_{row}^{1/2}x, (D_{row}^{1/2}CD_{col}^{-1/2} - Σ_i=0^{k-1} s_i v_i u_i^T)(D_{col}^{1/2}y)).

Here the upper bound is very close to 2∥(x, Ey)∥. The problem is that 
⟨1_{X}, Ey⟩ cannot be directly related to the discrepancy, like ⟨1_{X}, F y⟩. 
However, F and E are very ‘close’ to each other, since comparing Formulas (5) and (11), the difference between the corresponding entries of the 
block-matrices R and C is

|ρ(R_a, C_b) - ˆc_{ab}| = \frac{1}{\text{Vol}(R_a)\text{Vol}(C_b)} \left| \sum_{i \in R_a} \sum_{j \in C_b} \eta_{ij} \right|,

which is the density of the error matrix E = (η_{ij}) between R_a and C_b. If 
is this small enough, we may expect a finer upper estimate for s_k, based 
on E.

• Finally, note that C_{nor} corresponds to the linear operator taking conditional 
expectation between the margins of C and is widely used in multivariate statistics, namely, in correspondence analysis (see [4] for details). 
In the symmetric scenario [5], we considered a convergent sequence of edge-weighted graphs G^{(n)} = (V^{(n)}, W^{(n)}) and proved that for any fixed integer k > 0, s_i^{(n)} → s_i (i = 1, 2, . . . , k) as n → ∞, where s_i^{(n)} is the ith largest non-trivial singular value of W_{nor}^{(n)}, and s_i is the analogous singular value of the compact operator assigned to the limiting graphon, see Borgs et al. [8]. Since the singular values of a compact operator tend to 0 (s_k → 0), and the estimates of the forward and backward statements (see Theorem 1) do not depend on the size of the graph, there is a hope that to given α we can find a unique (possibly immensely large) k such that the k-way discrepancy of any sufficiently large weighted graph (in a convenient k-partition of its vertices) is at most α. This could be some spectral evidence of the Regularity Lemma [15].
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