When the largest eigenvalue of the modularity and the normalized modularity matrix is zero

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Abstract

In July 2012, at the Conference on Applications of Graph Spectra in Computer Science, Barcelona, D. Stevanovic posed the following open problem: which graphs have the zero as the largest eigenvalue of their modularity matrix? The conjecture was that only the complete and the complete multipartite graphs. They indeed have this property, but are they the only ones? In this paper, we will give an affirmative answer to this question and prove a bit more: both the modularity and the normalized modularity matrix of a graph is negative semidefinite if and only if the graph is complete or complete multipartite.

Keywords: Modularity matrix; Complete multipartite graphs; Normalized modularity; Modularity and Laplacian spectra.

1 Introduction

In [9] Newman and Girvan defined the modularity matrix of a simple graph on $n$ vertices with an $n \times n$ symmetric adjacency matrix $A$ as

$$M = A - \frac{1}{2e}dd^T,$$

where $d = (d_1, \ldots, d_n)^T$ is the so-called degree-vector comprised of the vertex-degrees $d_i$’s and $2e = \sum_{i=1}^{n} d_i$ is twice the number of edges. In [4] we formulated the modularity matrix of an edge-weighted graph $G = (V, W)$ on the $n$-element vertex-set $V$ with an $n \times n$ symmetric weight-matrix $W$ – the entries of which are pairwise similarities between the vertices and satisfy $w_{ij} = w_{ji} \geq 0$, $w_{ii} = 0$ ($i = 1, \ldots, n$), further, $\sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} = 1$ – as follows.

$$M = W - dd^T,$$
where the entries of \( d \) are now the generalized vertex-degrees \( d_i = \sum_{j=1}^{n} w_{ij} \) \( (i = 1, \ldots, n) \). The assumption \( \sum_{i=1}^{n} d_i = 1 \) does not hurt the generality, but simplifies further notation and makes it possible to consider \( W \) as a symmetric joint distribution of two identically distributed discrete random variables taking on \( n \) different values. The modularity matrix \( M \) always has a zero eigenvalue with eigenvector \( 1 = 1_n = (1, \ldots, 1)^T \), since its rows sum to zero. Because \( \text{tr}(M) < 0 \), \( M \) must have at least one negative eigenvalue, and it is usually indefinite. For the complete and the complete multipartite graphs, however, its largest eigenvalue is zero, as we will show in Section 3. In Theorem 1 of Section 4, we will prove that the modularity matrix of a simple graph is negative semidefinite if and only if it is complete or complete multipartite. In Theorem 2 we will extend this statement to the negative semidefiniteness of the normalized modularity matrix introduced in [4] as

\[
M_D = D^{-1/2}MD^{-1/2},
\]

where \( D = \text{diag}(d_1, \ldots, d_n) \) is the degree-matrix. The eigenvalues of \( M_D \) are the same, irrespective of whether we start with the adjacency or normalized edge-weight matrix of a simple graph, and they are in the \([-1, 1]\) interval. \( M_D \) is closely related to the normalized Laplacian; therefore, our statements have important consequences, as established in Section 2, for the normalized Laplacian spectrum. In Section 5, we discuss some other implications of Theorems 1 and 2 concerning the Newman–Girvan modularity of [9, 10] and the maximal correlation of [2].

## 2 Preliminaries

First we introduce some notation.

**Definition 1** The simple graph on \( n \) vertices is complete if the en-
tries of its adjacency matrix are

\[ a_{ij} := \begin{cases} 1 & \text{if } i \neq j \\ 0 & \text{if } i = j. \end{cases} \]

This graph is denoted by \( K_n \).

**Definition 2** The simple graph on the \( n \)-element vertex-set \( V \) is complete multipartite with \( 2 \leq k \leq n \) partites (color-classes) \( V_1, \ldots, V_k \) (they form a partition of the vertices) if the entries of its adjacency matrix are

\[ a_{ij} := \begin{cases} 1 & \text{if } c(i) \neq c(j) \\ 0 & \text{if } c(i) = c(j), \end{cases} \]

where \( c(i) \) is the color of vertex \( i \). Here the non-empty, disjoint vertex-subsets form so-called maximal independent sets of the vertices. If \( |V_i| = n_i \ (i = 1, \ldots, k), \sum_{i=1}^{k} n_i = n, \) then this graph is denoted by \( K_{n_1, \ldots, n_k} \).

Note that \( K_n \) is also complete multipartite with \( n \) partites, i.e., it is the \( K_{1, \ldots, 1} \) graph; therefore, in the sequel, whenever we speak of complete multipartite graphs, complete graphs are also understood.

In [1] we introduced the normalized Laplacian of \( G = (V, W) \) as \( L_D = I - D^{-1/2}WD^{-1/2} \), and in [4, 5] we established the following relation between the spectra of \( L_D \) and \( M_D \) when \( G \) is connected (\( W \) is irreducible). Let \( 0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2 \) denote eigenvalues of \( L_D \) with corresponding unit-norm, pairwise orthogonal eigenvectors \( u_0, \ldots, u_{n-1} \). Namely, \( u_0 = (\sqrt{d_1}, \ldots, \sqrt{d_n})^T \), which will be denoted by \( \sqrt{d} \). Enumerating the eigenvalues of \( M_D \) of the same connected graph in the order \( 1 > \mu_1 \geq \cdots \geq \mu_{n-1} \geq -1 \), we have \( \mu_i = 1 - \lambda_i \) with the same eigenvector \( u_i \ (i = 1, \ldots, n - 1) \); further, \( \mu_n = 0 \) with corresponding unit-norm eigenvector \( \sqrt{d} \).
The smallest positive normalized Laplacian eigenvalue $\lambda_1$ solves the following quadratic placement problem:

$$\lambda_1 = \min \sum_{i<j} w_{ij}(r_i - r_j)^2 \quad (1)$$

subject to

$$\sum_{i=1}^{n} d_i r_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} d_i r_i^2 = 1. \quad (2)$$

In [1] we proved that the optimal vertex-representatives $r_1, \ldots, r_n$ giving the above minimum are the coordinates of the vector $D^{-1/2}u_1$.

**Proposition 1** Let $G = (V, W)$ be an edge-weighted graph, the weight-matrix of which has at least one off-diagonal zero entry. Then $\lambda_1(G) \leq 1$.

**Proof:** Since the normalized Laplacian spectrum of isomorphic graphs is the same (irrespective of the same permutation of the rows and columns of $W$), we may assume that $w_{12} = 0$. Let us define the following representation of the vertices:

$$r_1 := \frac{d_2}{\sqrt{d_2^2d_1 + d_1^2d_2}}, \quad r_2 := -\frac{d_1}{\sqrt{d_2^2d_1 + d_1^2d_2}},$$

and $r_i := 0$, $i = 3, \ldots, n$ when $n$ exceeds 2. These representatives satisfy conditions (2) and in view of (1):

$$\lambda_1(G) \leq \sum_{i<j} (r_i - r_j)^2 w_{ij} = \frac{\sum_{j \neq 1} (d_2 - 0)^2 w_{1j} + \sum_{j \neq 2} (-d_1 - 0)^2 w_{2j}}{d_2^2d_1 + d_1^2d_2} = 1,$$

which finishes the proof.

We know (see e.g., [6]) that $\lambda_1(K_n) = \cdots = \lambda_{n-1}(K_n) = \frac{n}{n-1}$. Proposition 1 guarantees that all the other simple graphs have $\lambda_1 \leq 1$. This was also proved in [7]. In Section 4 we will prove that equality is attained only for $K_{n_1, \ldots, n_k}$ ($k < n$).
3 Modularity spectra of complete and complete multipartite graphs

Here we calculate modularity spectra of the exceptional graphs in question.

**Proposition 2** The spectrum of $M(K_n)$ consists of the single eigenvalue 0 with eigenvector $1_n$ and the number $-1$ with multiplicity $n-1$ and eigen-subspace $1_n^\perp$.

**Proof**: The adjacency matrix of $K_n$ is $A(K_n) = 1_n1_n^T - I_n$, $d = (n-1)1_n$, $2e = n(n-1)$, hence

$$M(K_n) = \frac{1}{n}1_n1_n^T - I_n = (\frac{1}{\sqrt{n}})(\frac{1}{\sqrt{n}})^T - \left[(\frac{1}{\sqrt{n}})(\frac{1}{\sqrt{n}})^T + \sum_{i=2}^{n} 1 \cdot u_iu_i^T\right]$$

$$= \sum_{i=2}^{n} (-1) \cdot u_iu_i^T,$$

where $u_2, \ldots u_n$ is an arbitrary orthonormal set in $1_n^\perp$. Therefore, the unique spectral decomposition of $M(K_n)$ is as stated in the proposition.

**Proposition 3** The spectrum of $M_D(K_n)$ consists of the single eigenvalue 0 with eigenvector $\sqrt{d}$ and the number $-\frac{1}{n-1}$ with multiplicity $n-1$ and eigen-subspace $\sqrt{d}^\perp$.

This proposition follows from the characterization of the normalized Laplacian spectrum of $K_n$ given in [6].

**Proposition 4** The spectrum of $M(K_{n_1, \ldots, n_k})$ consists of $k-1$ strictly negative eigenvalues and zero with multiplicity $n-k+1$.

**Proof**: The adjacency matrix $M$ of the complete multipartite graph $K_{n_1, \ldots, n_k}$ is a block-matrix with diagonal blocks of all zeros and off-diagonal blocks of all 1’s. Let $V_1, \ldots, V_k$ denote the independent,
disjoint vertex-subsets, $|V_i| = n_i$, $i = 1, \ldots, k$; $d_l = n - n_i$ if $l \in V_i$;
$2e = \sum_{l=1}^n d_l = \sum_{i=1}^k n_i(n - n_i) = n^2 - \sum_{i=1}^k n_i^2$. Therefore, $M$ is a blown-up matrix (see [6]) with blow-up sizes $n_1, \ldots, n_k$ of the $k \times k$ pattern matrix $P$ with entries

$$p_{ij} = (1 - \delta_{ij}) - \frac{(n - n_i)(n - n_j)}{2e},$$

where $\delta_{ij}$ is the Kronecker-delta. Consequently, rank($M$) = rank($P$) $\leq k$. We will prove that its rank is $k - 1$, it has $k - 1$ negative eigenvalues, and all its other eigenvalues are zeros. An eigenvector $u$ belonging to a nonzero eigenvalue $\lambda$ is piecewise constant with $n_1$ coordinates equal to $y_1, \ldots, n_k$ coordinates equal to $y_k$. With these, the eigenvalue–eigenvector equation yields that

$$\sum_{j=1}^k n_j \left[ (1 - \delta_{ij}) - \frac{(n - n_i)(n - n_j)}{2e} \right] y_j = \lambda y_i.$$

Therefore, $\lambda$ is an eigenvalue of the $k \times k$ matrix $PN$ with eigenvector $(y_1, \ldots, y_k)^T$, where $N = \text{diag}(n_1, \ldots, n_k)$. The matrix $PN$ is not symmetric, but its eigenvalues are real because of the above, or else its eigenvalues are also eigenvalues of the symmetric matrix $N^{1/2}PN^{1/2}$. It is easy to see that the row sums of $PN$ are zeros:

$$\sum_{j=1}^k n_j \left[ (1 - \delta_{ij}) - \frac{(n - n_i)(n - n_j)}{2e} \right] = 0,$$

i.e.,

$$\sum_{j=1}^k n_j p_{ij} y_j = \lambda y_i. \quad (3)$$

Therefore, zero is an eigenvalue with eigenvector $1_k$, which gives another zero eigenvalue of $M$ with eigenvector $1_n$. Thus, zero is an eigenvalue of $M$ with multiplicity $n - k + 1$ and corresponding eigensubspace of this dimension, including $1_n$. 

6
Now we will prove that all the non-zero eigenvalues are negative. In view of (3),
\[ \lambda \sum_{i=1}^{k} n_i y_i = \sum_{i=1}^{k} n_i (\lambda y_i) = \sum_{j=1}^{k} n_j y_j \sum_{i=1}^{k} n_i p_{ij} = 0. \]

Consequently, if \( \lambda \neq 0 \), then \( \sum_{i=1}^{k} n_i y_i = 0 \). On the other hand,
\[ \lambda \sum_{i=1}^{k} n_i y_i^2 = \sum_{i=1}^{k} (n_i y_i)(\lambda y_i) = \sum_{i=1}^{k} n_i y_i \sum_{j=1}^{k} p_{ij} n_j y_j = \sum_{i=1}^{k} \sum_{j=1}^{k} p_{ij}(n_i y_i)(n_j y_j). \]

We will show that the right hand side is negative, and therefore, by \( \sum_{i=1}^{k} n_i y_i^2 > 0 \), we get that \( \lambda < 0 \). Indeed,
\[
\sum_{i=1}^{k} \sum_{j=1}^{k} p_{ij}(n_i y_i)(n_j y_j) = \sum_{i=1}^{k} \sum_{j=1}^{k} \left[ (1 - \delta_{ij}) - \frac{(n - n_i)(n - n_j)}{2e} \right] (n_i y_i)(n_j y_j)
\]
\[
= \sum_{i=1}^{k} \sum_{j=1}^{k} (1 - \delta_{ij})(n_i y_i)(n_j y_j) - \frac{1}{2e} \left[ \sum_{i=1}^{k} (n - n_i)n_i y_i \right] \left[ \sum_{j=1}^{k} (n - n_j)n_j y_j \right]
\]
\[
= \left( \sum_{i=1}^{k} n_i y_i \right) \left( \sum_{j=1}^{k} n_j y_j \right) - \sum_{i=1}^{k} (n_i y_i)^2 - \frac{1}{2e} \left[ \sum_{i=1}^{k} (n - n_i)n_i y_i \right]^2 < 0,
\]

which, by \( \sum_{i=1}^{k} n_i y_i = 0 \), finishes the proof.

**Proposition 5** \( M_D(K_{n_1,\ldots,n_k}) \) is also negative semidefinite.

**Proof:** We have to show that for any \( x \in \mathbb{R}^n \), \( x^T M_D x \) is non-positive, where for brevity, \( M_D \) denotes the normalized modularity matrix of \( K_{n_1,\ldots,n_k} \). In fact,
\[
x^T M_D x = (D^{-1/2}x)^T M(D^{-1/2}x) = y^T M y \leq 0
\]
for any \( y \in \mathbb{R}^n \) because of the negative semidefiniteness of the modularity matrix of \( K_{n_1,\ldots,n_k} \). Due to the invertibility of the degree-matrix \( D \) (our graph is connected, hence cannot have isolated vertices), the above relation holds for any \( x \) as well.
Furthermore, $M_D(K_{n_1,\ldots, n_k})$ has rank $k - 1$ with $k - 1$ strictly negative eigenvalues, and the $(n - k + 1)$-dimensional eigensubspace corresponding to the zero eigenvalue looks like

$$\{\mathbf{x} : \sum_{j \in V_i} \sqrt{d_j}x_j = 0, i = 1, \ldots, k\} = \{\mathbf{x} : \sum_{j \in V_i} x_j = 0, i = 1, \ldots, k\}.$$ (4)

We can use that the vertex-degrees within the partites are the same, and so, we have a blown-up matrix again.

Note that in the case of $k = n$, the results of Propositions 4 and 5 exactly provide those of Propositions 2 and 3.

4 The main results and proofs

To prove the main results, we will intensively use the following characterization of complete multipartite graphs, including the complete graph. Although this is a known result of graph theory, we enclose the proof as well.

**Lemma 1** A simple connected graph is complete multipartite if and only if it has no 3-vertex induced subgraph with exactly one edge.

**Proof:** We will call the above subgraph *forbidden pattern*.

- In the forward direction, a complete multipartite graph can have the following types of 3-vertex induced subgraphs (not all of them appear necessarily, only if the size of partites allows it):
  - the three vertices are from the same partite, in which case the induced subgraph has no edges;
  - the three vertices are from three different partites, in which case the induced subgraph is the complete graph $K_3$;
  - two of the vertices are from the same, and the third from a different partite, in which case the induced subgraph has exactly two edges (called cherry).
None of them is the forbidden pattern.

- Conversely, suppose that our graph does not have the forbidden pattern. The following procedure shows that it is then complete multipartite. Let the first cluster be a maximal independent set of the vertices, say $V_1$. We claim that each vertex in $\overline{V}_1$ is connected to each vertex of $V_1$. Indeed, let $c \in \overline{V}_1$ be a vertex; it must be connected to a vertex (say, $a$) of $V_1$, since if not, it could be joined to $V_1$, which contradicts the maximality of $V_1$ as an independent set. If $c$ were not connected to another $b \in V_1$, then $a, b, c$ would form a forbidden pattern, but our graph does not contain such in view of our starting assumption.

Then let $V_2$ be a maximal independent set of vertices within $\overline{V}_1$, say $V_2$. We claim that each vertex in $\overline{V}_1 \cup \overline{V}_2$ is connected to each vertex of $V_1$ and $V_2$. The connectedness to vertices of $V_1$ is already settled. By the maximality of $V_2$ as an independent set, any vertex of $\overline{V}_1 \cup \overline{V}_2$ must be connected to at least one vertex of $V_2$. If we found a vertex $c \in \overline{V}_1 \cup \overline{V}_2$ such that for some $a \in V_2$: $a \sim c$, and for another $b \in V_2$: $b \not\sim c$, then $a, b, c$ would form a forbidden pattern, which is excluded.

Advancing in this way, one can see that the procedure produces maximal disjoint independent sets of vertices such that the independent vertices of $V_k$ are connected to every vertex in $V_1, \ldots, V_{k-1}$. At each step we can select a maximal independent set out of the remaining vertices; in the worst case it contains only one vertex. The absence of the forbidden pattern guarantees that we can always continue our algorithm until all vertices are placed into a cluster. This procedure will exhaust the set of vertices and result in a complete multipartite graph. The point is that in the absence of the forbidden pattern we can divide the vertices into independent sets which are fully connected.
If we proceed with non-increasing cardinalities of $V_i$’s, then one-vertex independent sets may emerge at the end of the process. Moreover, up to the labeling of the vertices and the numbering of the independent sets, the resulting multipartite structure is unique. In fact, the above procedure just recovers this unique structure in the absence of the forbidden pattern.

Now, the answer to the open question follows.

**Theorem 1** The modularity matrix of a simple connected graph is negative semidefinite if and only if it is complete multipartite.

**Proof:** First we prove that when a simple graph is not complete multipartite, then its modularity matrix cannot be negative semidefinite. By Lemma 1, a simple graph is not complete multipartite if and only if it contains the forbidden pattern. Let us take such a graph. Since the modularity spectrum does not depend on the labeling of the vertices, assume that the first three vertices form the forbidden pattern, i.e., the upper left corner of the adjacency matrix is

$$
\begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
$$

It is known that a matrix is negative semidefinite if and only if its every principal minor of odd order is non-positive, and every principal minor of even order is non-negative. Since the principal minor of order 3 of this graph’s modularity matrix is

$$
(\frac{1}{2e})^3 \det \begin{pmatrix}
-d_1^2 & 2e - d_1 d_2 & -d_1 d_3 \\
2e - d_1 d_2 & -d_2^2 & -d_2 d_3 \\
-d_1 d_3 & -d_2 d_3 & -d_3^2
\end{pmatrix} = \frac{1}{8e^3} 4e^2 d_3^2 = \frac{d_3^2}{2e} > 0,
$$

the modularity matrix cannot be negative semidefinite. This fact, together with Proposition 4, finishes the proof.

We are able to prove a similar statement for the normalized modularity matrix.
Theorem 2 The normalized modularity matrix of a simple connected graph is negative semidefinite if and only if it is complete multipartite.

Proof: Now we will prove that if a simple graph is not complete multipartite, or equivalently, if it contains the forbidden pattern, then the largest eigenvalue of its normalized modularity matrix is strictly positive. This fact, together with Proposition 5, will finish the proof.

Referring to [5], the largest eigenvalue $\mu_1$ of $M_D$ is the second largest eigenvalue of $D^{-1/2}WD^{-1/2}$, whose largest eigenvalue is 1 with corresponding eigenvector $\sqrt{d}$ (this is unique if our graph is connected). Therefore, we think in terms of the two largest eigenvalues of $D^{-1/2}WD^{-1/2}$. We can again assume that the first three vertices form the forbidden pattern and so, the upper left corner of this matrix looks like

$$
\begin{pmatrix}
0 & \frac{1}{\sqrt{d_1d_2}} & 0 \\
\frac{1}{\sqrt{d_1d_2}} & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}.
$$

Then by the Courant–Fischer–Weyl minimax principle:

$$
\mu_1 = \max_{\|x\|=1, \ x^T\sqrt{d}=0} x^TD^{-1/2}WD^{-1/2}x.
$$

Therefore, to prove that $\mu_1 > 0$, it suffices to find an $x \in \mathbb{R}^n$ ($n$ is the number of vertices) that satisfies conditions $\|x\| = 1$, $x^T\sqrt{d} = 0$ and for which $x^TD^{-1/2}WD^{-1/2}x > 0$. (The unit norm condition can be relaxed here, because $x$ can later be normalized, without changing the sign of the above quadratic form.) Indeed, let us look for $x$ in the form $x = (x_1, x_2, x_3, 0, \ldots, 0)^T$ such that

$$
\sqrt{d_1}x_1 + \sqrt{d_2}x_2 + \sqrt{d_3}x_3 = 0. \tag{5}
$$
Then the inequality
\[ x^T M_D x = \frac{2x_1x_2}{\sqrt{d_1d_2}} > 0 \]
can be satisfied with any \( x = (x_1, x_2, x_3, 0, \ldots, 0)^T \) such that \( x_1 \) and \( x_2 \) are both positive or both negative, and due to (5),
\[ x_3 = -\frac{\sqrt{d_1x_1} + \sqrt{d_2x_2}}{\sqrt{d_3}} \]
is a good choice, which will have the opposite sign. (Note that \( d_i \)'s are positive, since we deal with connected graphs.)

5 Conclusions

The results of Section 4 have the following important implications.

- In terms of \( \mu_1 \), a result of [2] can be interpreted in the following way. We use the setup of correspondence analysis, applied to the symmetric joint distribution embodied by the entries of \( W \). Let \( \psi \) and \( \phi \) be identically distributed (i.d.) random variables with this joint distribution. Say, these discrete random variables take on values \( r_1, \ldots, r_n \) with probabilities \( d_1, \ldots, d_n \) (margin of the joint distribution; the two margins are the same, since \( W \) is symmetric). Then

\[
\mu_1 = \max_{\psi, \phi \text{ i.d.}} \text{Corr}_W(\psi, \phi) = \max_{\psi, \phi \text{ i.d.}} \text{Cov}_W(\psi, \phi) = \max_{\sum_{i=1}^n d_ir_i = 0 \atop \sum_{i=1}^n d_ir_i^2 = 1} \sum_{i=1}^n \sum_{j=1}^n w_{ij} r_i r_j,
\]

and the maximum is attained when the values \( r_1, \ldots, r_n \) are coordinates of the vector \( D^{-1/2}u_1 \). In this setup, the conditions for the zero expectation and unit variance are analogous to those of (2). In [2] \( \mu_1 \) is called symmetric maximal correlation. The results of the present paper show that it is positive if and only if the joint distribution is not of a complete multipartite structure.
The 2-way Newman–Girvan modularity (see [9, 10, 4]) of \( G = (V, W) \) is

\[
Q_2 = \max_{\emptyset \neq U \subset V} Q(U, \overline{U}),
\]

where the modularity of the 2-partition \((U, \overline{U})\) of \( V \) is written in terms of the entries \( m_{ij} \)'s (summing to 0) of \( M(G) \):

\[
Q(U, \overline{U}) = \sum_{i,j \in U} m_{ij} + \sum_{i,j \in \overline{U}} m_{ij} = -2 \sum_{i \in U, j \in \overline{U}} m_{ij}
\]

\[
= -2[w(U, \overline{U}) - \text{Vol}(U)\text{Vol}(\overline{U})],
\]

where \( w(U, \overline{U}) = \sum_{i \in U} \sum_{j \in \overline{U}} w_{ij} \) is the weighted cut between \( U \) and \( \overline{U} \), whereas \( \text{Vol}(U) = \sum_{i \in U} d_i \) is the volume of the vertex-subset \( U \). These formulas are valid under the condition \( \text{Vol}(V) = 1 \); otherwise, they should be adjusted by \( 2e \).

Now we use the idea of the proof of the Expander Mixing Lemma extended to edge-weighted graphs (see [5]).

With the notation of Section 2 and introducing \( \mu_0 = 1, u_0 = \sqrt{d}, \)

\[
D^{-1/2}WD^{-1/2} = \sum_{i=0}^{n-1} \mu_i u_i u_i^T
\]

is spectral decomposition.

Let \( U \subset V \) be arbitrary and the indicator vector of \( U \) is denoted by \( \mathbf{1}_U \in \mathbb{R}^n \). Further, put \( \mathbf{x} := D^{1/2}\mathbf{1}_U \) and \( \mathbf{y} := D^{1/2}\mathbf{1}_{\overline{U}} \), and let \( \mathbf{x} = \sum_{i=0}^{n-1} a_i u_i \) and \( \mathbf{y} = \sum_{i=0}^{n-1} b_i u_i \) be the expansions of \( \mathbf{x} \) and \( \mathbf{y} \) in the orthonormal basis \( u_0, \ldots, u_{n-1} \) with coordinates \( a_i = \mathbf{x}^T u_i \) and \( b_i = \mathbf{y}^T u_i \), respectively. Observe that \( w(U, \overline{U}) = \mathbf{1}_U^T \mathbf{W} \mathbf{1}_{\overline{U}} = \mathbf{x}^T (D^{-1/2}WD^{-1/2}) \mathbf{y}^T \) and \( \mathbf{1}_{\overline{U}} = \mathbf{1}_n - \mathbf{1}_U \); therefore,

\[
b_i = \mathbf{y}^T u_i = D^{1/2}(1 - \mathbf{1}_U) u_i = u_0^T u_i - \mathbf{x}^T u_i = -a_i (i = 1, 2, \ldots, n-1).
\]
Further, $a_0 = \text{Vol}(U)$ and $b_0 = \text{Vol}(\overline{U})$. Based on these observations,

$$w(U, \overline{U}) - \text{Vol}(U)\text{Vol}(\overline{U}) = \sum_{i=1}^{n-1} \mu_i a_i b_i = -\sum_{i=1}^{n-1} \mu_i a_i^2.$$  

Consequently, $Q(U, \overline{U}) = 2 \sum_{i=1}^{n-1} \mu_i a_i^2$. Therefore, provided that the normalized modularity matrix of the underlying graph is negative semidefinite (or equivalently, our graph is complete multipartite), $Q(U, \overline{U}) \leq 0$ for all 2-partitions of the vertices, and hence, the 2-way Newman–Girvan modularity is also non-positive (in most cases, it is negative). Nonetheless this property does not characterize the complete multipartite graphs. There are graphs with positive $\mu_1$ and zero or sometimes negative 2-way Newman–Girvan modularity.

• Recall that the smallest positive normalized Laplacian eigenvalue $\lambda_1$ is slightly greater than 1 for complete, equal to 1 for complete multipartite, and strictly less than 1 for other graphs. In the case of $\lambda_1 < 1$ we gave an upper and lower estimate for the Cheeger constant of the graph by $\lambda_1$ (see [2]), illustrating that a smallest positive normalized Laplacian eigenvalue a separated from zero is an indication of the high edge-expansion of the graph. In view of the above, this estimation is not valid for complete and complete bipartite or multipartite graphs. Indeed, former ones are, in fact, super-expanders, while latter ones are so-called bipartite or multipartite expanders. By continuity, for large $n$, a $\lambda_1$ close to 1 (from the left) is also ‘suspicious’, as it may indicate that our graph is close to a bipartite or multipartite expander. The situation can even be more complicated and also influenced by the upper end (near to 2 eigenvalues) of the normalized Laplacian matrix, see [6].
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