SPECTRAL CLUSTERING, Lesson 3.

Normalized cuts, modularity cuts, isoperimetric number, bicuts

Marianna Bolla, DSc. Prof. BME Math. Inst.

October 1, 2020

Normalized multiway cut problems are discussed together with modularity cuts. Since the optima of the corresponding objective functions are taken on partition vectors corresponding to the hidden clusters, they are related to Laplacian, normalized Laplacian, or modularity spectra, whereas the precision of the estimates depends on the distance between the subspaces spanned by the corresponding eigenvectors and partition vectors. By an Analysis of Variance argument, this distance is the sum of the inner variances of the underlying clusters, the objective function of the k-means clustering.

Clusters (in other words, modules or communities) of graphs are typical (strongly or loosely connected) subsets of vertices that can be identified, for example, with social groups or interacting enzymes in social or metabolic networks, respectively; they form special partition classes of the vertices. To measure the performance of a clustering, different kinds of multiway cuts are introduced and estimated by means of Laplacian spectra. The key motif of these estimations is that minima and maxima of the quadratic placement problems are attained on some appropriate eigenspaces of the Laplacian, while optimal multiway cuts are special values of the same quadratic objective function realized by piecewise constant vectors. Hence, the optimization problem, formulated in terms of the Laplacian eigenvectors, is the continuous relaxation of the underlying maximum or minimum multiway cut problem. The objective functions defined on the partitions of the vertices are sometimes called modularities, see [58, 63].

1 Normalized cuts

Here we will use the normalized Laplacian matrix to find so-called minimum normalized cuts of edge-weighted graphs. Normalized cuts also favor balanced partitions, but the balancing is in terms of the cluster-volumes defined by the generalized degrees.

Definition 1 *Let $G = (V, \boldsymbol{W})$ be an edge-weighted graph with generalized degrees $d_1, \dots, d_n$ and assume that $\sum_{i=1}^n d_i = 1$. For the vertex-subset $U \subset V$ let $\mathrm{Vol}(U) = \sum_{i \in U} d_i$ denote the volume of U. The k-way normalized cut of G*

corresponding to the k-partition $P_k = (V_1, \ldots, V_k)$ *of* V *is defined by*

$$\begin{aligned} f(P_k, G) &= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left(\frac{1}{\mathrm{Vol}(V_a)} + \frac{1}{\mathrm{Vol}(V_b)} \right) w(V_a, V_b) \\ &= \sum_{a=1}^{k} \frac{w(V_a, \overline{V}_a)}{\mathrm{Vol}(V_a)} = k - \sum_{a=1}^{k} \frac{w(V_a, V_a)}{\mathrm{Vol}(V_a)}. \end{aligned} \tag{1}$$

The minimum k-way normalized cut of G *is*

$$f_k(G) = \min_{P_k \in \mathcal{P}_k} f(P_k, G). \tag{2}$$

The equivalence of the seemingly different expressions in (1) can be easily verified, using that $\sum_{a=1}^{k} \mathrm{Vol}(V_a) = \sum_{i=1}^{n} d_i = 1$. It is easy to see that $f_k(G)$ punishes k-partitions with 'many' inter-cluster edges of 'large' weights and with 'strongly' differing volumes. The quantity $f_2(G)$ was introduced in [56] for simple graphs and in [54] for edge-weighted graphs; further, for a general k in [9] and [16], though they called it k-density of G.

Now, $f_k(G)$ will be related to the k smallest normalized Laplacian eigenvalues. Recall that the normalized Laplacian $\boldsymbol{L}_D$ (see Definition **??**) is unaffected by scaling the edge-weights, its spectrum is in the $[0, 2]$ interval and 0 is a single eigenvalue whenever G is connected.

Theorem 1 *Assume that* $G = (V, \boldsymbol{W})$ *is connected and let* $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$ *denote the eigenvalues of its normalized Laplacian matrix. Then*

$$\sum_{i=1}^{k-1} \lambda_i \leq f_k(G) \tag{3}$$

and in the case when the optimal k*-dimensional representatives of the vertices can be classified into* k *well-separated clusters* $V_1, \ldots, V_k$ *in such a way that the maximum cluster diameter* ε *satisfies the relation* $\varepsilon \leq \min\{1/\sqrt{2k}, \sqrt{2} \min_i \sqrt{p_i}\}$*, where* $p_i = \mathrm{Vol}(V_i)$*,* $i = 1, \ldots, k$*, then*

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

where $c = 1 + \varepsilon c'/(\sqrt{2} - \varepsilon c')$ *and* $c' = 1/\min_i \sqrt{p_i}$*.*

To prepare the proof, analogously to the balanced partition vectors, we will introduce the notion of the normalized partition vectors. The k-partition P_k is uniquely determined by the $n \times k$ normalized partition matrix $\boldsymbol{Z}_k = (\mathbf{z}_1, \ldots, \mathbf{z}_k)$, where the a-th *normalized k-partition vector* $\mathbf{z}_a = (z_{1a}, \ldots, z_{na})^T$ is the following:

$$z_{ia} = \begin{cases} \frac{1}{\sqrt{\mathrm{Vol}(V_a)}} & \text{if} \quad i \in V_a \\ 0 & \text{otherwise.} \end{cases} \tag{4}$$

The matrix $\boldsymbol{D}^{1/2}\boldsymbol{Z}_k$ is obviously suborthogonal, where $\boldsymbol{D}$ is the diagonal degree-matrix. The set of normalized k-partition matrices is denoted by $\mathcal{Z}_k^N$. The

normalized cut of $G = (V, \boldsymbol{W})$ corresponding to the k-partition P_k can be rewritten as

$$f(P_k, G) = \sum_{a=1}^{k} \mathbf{z}_a^T \boldsymbol{L} \mathbf{z}_a = \mathrm{tr}(\boldsymbol{Z}_k^T \boldsymbol{L} \boldsymbol{Z}_k) = \mathrm{tr}[(\boldsymbol{D}^{1/2}\boldsymbol{Z}_k)^T \boldsymbol{L}_D (\boldsymbol{D}^{1/2}\boldsymbol{Z}_k)] \quad (5)$$

and $f_k(G)$ is its minimum over $\mathcal{Z}_k^N$.

Proof 1 • *Lower bound. The discrete problem is again relaxed to a continuous one. Let $\tilde{\mathbf{r}}_1, \ldots, \tilde{\mathbf{r}}_n$ be k-dimensional representatives of the vertices subject to $\sum_{i=1}^n d_i \tilde{\mathbf{r}}_i \tilde{\mathbf{r}}_i^T = \boldsymbol{I}_k$. Let $\tilde{\boldsymbol{X}}$ denote the $n \times k$ matrix with these representatives as row-vectors. With the augmented $n \times k$ matrix $\tilde{\boldsymbol{X}}$,*

$$\begin{aligned} &\min_{\tilde{\boldsymbol{X}}^T \boldsymbol{D} \tilde{\boldsymbol{X}} = \boldsymbol{I}_k} \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} w_{ij} \|\tilde{\mathbf{r}}_i - \tilde{\mathbf{r}}_j\|^2 \\ &= \min_{\tilde{\boldsymbol{X}}^T \boldsymbol{D} \tilde{\boldsymbol{X}} = \boldsymbol{I}_k} \mathrm{tr}[(\boldsymbol{D}^{1/2}\tilde{\boldsymbol{X}})^T \boldsymbol{L}_D (\boldsymbol{D}^{1/2}\tilde{\boldsymbol{X}})] = \sum_{i=1}^{k-1} \lambda_i = \sum_{i=0}^{k-1} \lambda_i \end{aligned} \quad (6)$$

holds, and equality is attained with $\boldsymbol{X}^* = (\boldsymbol{D}^{-1/2}\mathbf{u}_0, \ldots, \boldsymbol{D}^{-1/2}\mathbf{u}_{k-1})$, where $\mathbf{u}_0, \ldots \mathbf{u}_{k-1}$ are unit-norm, pairwise orthogonal eigenvectors corresponding to the eigenvalues $\lambda_0, \ldots, \lambda_{k-1}$ of $\boldsymbol{L}_D$. We also saw that $\boldsymbol{D}^{-1/2}\mathbf{u}_0 = \mathbf{1}$.

Since the normalized k-partition matrix $\boldsymbol{Z}_k$ satisfies $\boldsymbol{Z}_k^T \boldsymbol{D} \boldsymbol{Z}_k = \boldsymbol{I}_k$, the equivalent form (5) for $f(P_k, G)$ implies that

$$f_k(G) = \min_{\boldsymbol{Z}_k \in \mathcal{Z}_k^N} \mathrm{tr}(\boldsymbol{Z}_k^T \boldsymbol{L} \boldsymbol{Z}_k) \geq \sum_{i=0}^{k-1} \lambda_i \quad (7)$$

and equality can be attained only in the $k = 1$ trivial case, otherwise the vectors $\boldsymbol{D}^{-1/2}\mathbf{u}_i$ cannot be normalized partition vectors, since any $\mathbf{u}_i$ $(i = 1, \ldots, k-1)$ has both positive and negative coordinates because of the orthogonality to the $\mathbf{u}_0 = \sqrt{\mathbf{d}}$ vector.

- *Upper bound. To effectuate the upper estimation, let $P_k = (V_1, \ldots, V_k)$ be a k-partition obtained by k-means classification of the optimal k-dimensional Euclidean vertex representatives, $\mathbf{r}_1^*, \ldots, \mathbf{r}_n^*$ (row vectors of $\boldsymbol{X}^*$ all having 1 as first coordinate). In fact, the clusters $V_1, \ldots, V_k$ are obtained by minimizing the weighted k-variance of these representatives. According to our assumption,*

$$\varepsilon = \max_{c(i)=c(j)} \|\mathbf{r}_i^* - \mathbf{r}_j^*\| \leq \min\{\frac{1}{\sqrt{2k}}, \sqrt{2} \min_i \sqrt{p_i}\},$$

where $c(i)$ denotes the cluster membership of vertex i. The representatives satisfy the condition $\sum_{j=1}^n d_j \mathbf{r}_j^* \mathbf{r}_j^{*T} = \boldsymbol{X}^* \boldsymbol{D} \boldsymbol{X}^{*T} = \boldsymbol{I}_k$.

Let $\bar{\mathbf{r}}^{(i)}$ denote the weighted center of the ith cluster:

$$\bar{\mathbf{r}}^{(i)} = \frac{1}{p_i} \sum_{j \in V_i} d_j \mathbf{r}_j^*, \quad i = 1, \ldots, k.$$

Further, let $\mathbf{y}_i$ *denote the* k*-dimensional vector with coordinates*

$$y_{ij} = \begin{cases} \frac{1}{\sqrt{p_i}} & \text{if} \quad j \in V_i \\ 0 & \text{otherwise} \end{cases}$$

and $\boldsymbol{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_k)$*. In fact, with* $\boldsymbol{P} = \mathrm{diag}(p_1, \ldots, p_k)$*, the relation* $\boldsymbol{Y} = \boldsymbol{P}^{-1/2}$ *holds. Let* $\boldsymbol{R}$ *be a* $k \times k$ *orthogonal matrix. With the notation* $\mathbf{y}'_i = \boldsymbol{R}\mathbf{y}_i$ *and* $\boldsymbol{Y}' = \boldsymbol{RY}$ *we are looking for a system* $\boldsymbol{Y}'$ *such that* $\mathbf{y}'_i$ *is 'close' to the cluster center* $\bar{\mathbf{r}}^{(i)}$ *for* $i = 1, \ldots, k$*. To this end, we use the a Multivariate Analysis of Variance (MANOVA) technique. We adopt the decomposition to the situation when the variances are calculated with respect to the degree distribution, i.e. we use the weights* $d_1, \ldots, d_n$ *in the formula. In this way, the* $k \times k$ *empirical covariance matrix of* $\mathbf{r}^*_j$*'s is decomposed into within-cluster and between-cluster covariances in the following way (the weighted mean of the coordinates of* $\mathbf{r}^*_j s$ *is zero except the first one that is identically 1, but it will not contribute to the variances):*

$$\sum_{j=1}^{n} d_j \mathbf{r}^*_j \mathbf{r}^{*T}_j = \sum_{i=1}^{k} \sum_{j \in V_i} d_j (\mathbf{r}^*_j - \bar{\mathbf{r}}^{(i)})(\mathbf{r}^*_j - \bar{\mathbf{r}}^{(i)})^T + \sum_{i=1}^{k} p_i \bar{\mathbf{r}}^{(i)} \bar{\mathbf{r}}^{(i)T}$$

or briefly,

$$\boldsymbol{I}_k = \sum_{i=1}^{k} \boldsymbol{A}_i + \boldsymbol{B} = \boldsymbol{A} + \boldsymbol{B}$$

where $\boldsymbol{A}_i = \sum_{j \in V_i} d_j (\mathbf{r}^*_j - \bar{\mathbf{r}}^{(i)})(\mathbf{r}^*_j - \bar{\mathbf{r}}^{(i)})^T$*,* $i = 1, \ldots, k$*. Here* $\mathrm{tr}(\boldsymbol{A}_i)$ *is the* k*-variance of representatives in cluster* i*, therefore* $\mathrm{tr}(\boldsymbol{A}_i) \leq \sum_{c(j)=i} d_j \varepsilon^2 = p_i \varepsilon^2$*, and* $\mathrm{tr}(\boldsymbol{A}) = \sum_{i=1}^{k} \mathrm{tr}(\boldsymbol{A}_i) \leq \varepsilon^2$*. Since* $\boldsymbol{A}$ *is symmetric, positive semidefinite, its maximum eigenvalue is at most* ε^2*. Hence,* $\boldsymbol{A}$ *will be viewed as a perturbation on* $\boldsymbol{B}$*. The matrix* $\boldsymbol{B} = \boldsymbol{I}_k - \boldsymbol{A}$ *is also positive semidefinite and by the Weyl's perturbation theorem for symmetric matrices it follows that denoting by* $\beta_1, \ldots \beta_k$ *its eigenvalues, for them the relation*

$$0 \leq 1 - \beta_i \leq \varepsilon^2, \qquad i = 1, \ldots, k$$

holds. With the notation $\bar{\boldsymbol{X}} = (\bar{\mathbf{r}}^{(1)}, \ldots, \bar{\mathbf{r}}^{(k)})$ *our matrix* $\boldsymbol{B}$ *is equal to* $\bar{\boldsymbol{X}} \boldsymbol{P} \bar{\boldsymbol{X}}^T$*.*

Now, let us find an $\boldsymbol{R}$ *such that, with* $(\mathbf{y}'_1, \ldots, \mathbf{y}'_k) = \boldsymbol{RY}$*, the sum* $\sum_{i=1}^{k} p_i \|\bar{\mathbf{r}}^{(i)} - \mathbf{y}'_i\|^2$ *be the least possible.*

$$\begin{aligned} &\sum_{i=1}^{k} p_i \|\bar{\mathbf{r}}^{(i)} - \mathbf{y}'_i\|^2 = \mathrm{tr}[(\bar{\boldsymbol{X}} - \boldsymbol{RY})\boldsymbol{P}(\bar{\boldsymbol{X}} - \boldsymbol{RY})^T] \\ &= \mathrm{tr}(\bar{\boldsymbol{X}} \boldsymbol{P} \bar{\boldsymbol{X}}^T) + \mathrm{tr}(\boldsymbol{RY} \boldsymbol{P} \boldsymbol{Y}^T \boldsymbol{R}^T) - 2\mathrm{tr}(\bar{\boldsymbol{X}} \boldsymbol{P} \boldsymbol{Y}^T \boldsymbol{R}) \qquad (8) \\ &\geq \sum_{i=1}^{k} \beta_i + k - 2 \sum_{i=1}^{k} s_i \end{aligned}$$

where $s_1, \ldots, s_k$ *are the singular values of the matrix* $\bar{\boldsymbol{X}} \boldsymbol{P} \boldsymbol{Y}^T$*. Indeed, the first term is* $\mathrm{tr}\boldsymbol{B}$*, the second is* $\mathrm{tr}\boldsymbol{I}_k$*, while to the third one Proposition* **??** *of the Appendix is applicable as follows. With our notation,* $\mathrm{tr}(\bar{\boldsymbol{X}} \boldsymbol{P} \boldsymbol{Y}^T \boldsymbol{R})$

is maximal (with respect to $\boldsymbol{R}$) if the matrix $\bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{Y}^T\boldsymbol{R}$ is symmetric and the maximum is equal to the sum of the singular values of $\bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{Y}^T$. By choosing such an $\boldsymbol{R}$, equality can be attained. Taking into consideration that

$$(\bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{Y}^T)(\bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{Y}^T)^T = \bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{Y}^T\boldsymbol{Y}\boldsymbol{P}\bar{\boldsymbol{X}}^T = \bar{\boldsymbol{X}}\boldsymbol{P}\boldsymbol{P}^{-1}\boldsymbol{P}\bar{\boldsymbol{X}}^T$$
$$= \bar{\boldsymbol{X}}\boldsymbol{P}\bar{\boldsymbol{X}}^T = \boldsymbol{B},$$

the eigenvalues of $\boldsymbol{B}$ can be enumerated in such a way that $\beta_i = s_i^2$, $i = 1, \ldots, k$. But we saw that s_i^2 is of order $1 - \varepsilon^2$, therefore, via Taylor's expansion, $1 - s_i \approx \dfrac{\varepsilon^2}{2} + \dfrac{\varepsilon^4}{4}$ is a good approximation. Hence, with the choice of $\boldsymbol{R}$ giving equality in (8) we have that

$$\sum_{i=1}^{k} p_i \|\bar{\mathbf{r}}^{(i)} - \mathbf{y}_i'\|^2 = \sum_{i=1}^{k} s_i^2 - k + 2k - 2\sum_{i=1}^{k} s_i$$
$$\sum_{i=1}^{k}(s_i^2 - 1) + 2\sum_{i=1}^{k}(1 - s_i) \approx 2k\varepsilon^4$$

that is less than ε^2 provided that $\varepsilon \leq 1/\sqrt{2k}$ holds. Consequently, $p_i\|\bar{\mathbf{r}}^{(i)} - \mathbf{y}_i'\|^2 \leq \varepsilon^2$ and $\|\bar{\mathbf{r}}^{(i)} - \mathbf{y}'\| \leq \varepsilon c'$.

Let the $\mathbf{y}_i'$ nearest to $\bar{\mathbf{r}}^{(i)}$ be denoted by $\mathbf{y}(\mathbf{r}_j^*)$ for every j in V_i (thus $\mathbf{y}(\mathbf{r}_j^*) = \mathbf{y}_i'$, $\forall\ j \in V_i$). Let δ denote the minimum distance between the different $\mathbf{y}_i'$'s, that is

$$\delta = \min_{a \neq b} \|\mathbf{y}_a' - \mathbf{y}_b'\| = \min_{a \neq b} \|\mathbf{y}_a - \mathbf{y}_b\| = \min_{a \neq b} \sqrt{\frac{1}{p_a} + \frac{1}{p_b}} \geq \sqrt{2}.$$

Then the estimation

$$f_k(G) \leq f_k(P_k, G) = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|\mathbf{y}(\mathbf{r}_i^*) - \mathbf{y}(\mathbf{r}_j^*)\|^2$$
$$\leq \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}(c\|r_i^* - r_j^*\|)^2 = c^2\sum_{i=1}^{k-1}\lambda_i$$

holds with the constant

$$c = \frac{\delta}{\delta - \varepsilon c'} = 1 + \frac{\varepsilon c'}{\delta - \varepsilon c'} \leq 1 + \frac{\varepsilon c'}{\sqrt{2} - \varepsilon c'}$$

where we used Equation (6) and the optimality of the representation $\mathbf{r}_1^*, \ldots, \mathbf{r}_n^*$. This finishes the proof.

Note that the constant c of the upper estimation is greater than 1, and it is the closer to 1, the smaller ε is. The latter requirement is satisfied if there exists a 'very' well-separated k-partition of the k-dimensional Euclidean representatives. From Theorem 1 we can also conclude that the gap in the spectrum is a necessary but not a sufficient condition of a good classification. In addition, the Euclidean representatives should be well classified in the appropriate dimension.

The following theorem directly estimates the weighted 2-variance of the optimal representatives of the vertices by the ratio of the two smallest positive normalized Laplacian eigenvalues.

Theorem 2 *Let $G = (V, \boldsymbol{W})$ be connected edge-weighted graph with generalized degrees $d_1, \ldots, d_n$ and assume that $\sum_{i=1}^n d_i = 1$. Let $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ denote the eigenvalues of the normalized Laplacian matrix of G. Then for the weighted 2-variance of the optimal vertex representatives, comprising row vectors of the matrix $\boldsymbol{X}_2^*$, the following upper estimate holds:*

$$\tilde{S}_2^2(\boldsymbol{X}_2^*) \leq \frac{\lambda_1}{\lambda_2}.$$

In main lines, we will follow the proof of [15]. Before plunging into it, let us recall that $\boldsymbol{X}_2^* = (\boldsymbol{D}^{-1/2}\mathbf{u}_0, \boldsymbol{D}^{-1/2}\mathbf{u}_1)$, where $\mathbf{u}_0$ and $\mathbf{u}_1$ are unit-norm, orthogonal eigenvectors corresponding to the eigenvalues λ_0 and λ_1 of $\boldsymbol{L}_D$, respectively. Because $\boldsymbol{D}^{-1/2}\mathbf{u}_0$ is the $\mathbf{1}$ vector, the first column of $\boldsymbol{X}_2^*$ can as well be omitted in the representation and we only use the coordinates of the vector $\mathbf{x}^* := \boldsymbol{D}^{-1/2}\mathbf{u}_1 = (x_1^*, \ldots, x_n^*)$. Therefore,

$$s^2 = \tilde{S}_2^2(\boldsymbol{X}_2^*) = \min_{\substack{c(i)\in\{1,2\},\, i=1,\ldots,n \\ m_1, m_2}} \sum_{i=1}^n d_i (x_i^* - m_{c(i)})^2, \tag{9}$$

where the minimization over the 2-partitions of V is uniquely defined by the cluster memberships $c(i)$'s of the vertices ($c(i) = 1$ or $c(i) = 2$ depending on whether vertex i corresponds to the first or second cluster), and the cluster centers are $m_1, m_2 \in \mathbb{R}$.

Proof 2 *As $\mathbf{u}_1$ is the unit-norm vector and orthogonal to the $\mathbf{u}_0 = \sqrt{\mathbf{d}}$ vector, for the coordinates of $\mathbf{x}^*$ the following relations hold:*

$$\sum_{i=1}^n d_i x_i^* = 0 \quad \textit{and} \quad \sum_{i=1}^n d_i x_i^{*2} = 1. \tag{10}$$

Now we will find a vector $\mathbf{y} = (y_1, \ldots, y_n)$ such that for it, the conditions

$$\sum_{i=1}^n d_i y_i = 0 \tag{11}$$

and

$$\sum_{i=1}^n d_i x_i^* y_i = 0 \tag{12}$$

are met. We are looking for $\mathbf{y}$ in the following form:

$$y_i := |x_i^* - a| - b, \quad (i = 1, \ldots, n) \tag{13}$$

where a and b are appropriate real numbers.

We will show that there exist real numbers a and b such that the y_i's defined by them satisfy conditions (11) and (12). Indeed, when we already have a, the above conditions together with $\sum_{i=1}^n d_i = 1$ yield

$$b = \sum_{i=1}^n d_i |x_i^* - a| \tag{14}$$

for b. With this choice of b, the fulfillment of (12) means that

$$\sum_{i=1}^{n} d_i x_i^* |x_i^* - a| = 0.$$

Since the left-hand side of the above equation is a continuous function of a, and it is equal to 1 if $a \leq \min_i x_i^*$, and -1 if $a \geq \max_i x_i^*$, by the Bolzano—Weierstrass theorem, the function $\sum_{i=1}^{n} d_i x_i^* |x_i^* - a|$ must have a root (in a) somewhere between $\min_i x_i^*$ and $\max_i x_i^*$. Choosing such an a and the corresponding b via (14), the coordinates of $\mathbf{y}$ are then uniquely determined by (13). Let us define the cluster centers by

$$m_1 = a - b \quad \textit{and} \quad m_2 = a + b.$$

It is easy to see that

$$y_i = |x_i^* - a| - b = \begin{cases} m_1 - x_i^* & \textit{if} \quad x_i^* < a \\ x_i^* - m_2 & \textit{if} \quad x_i^* \geq a, \end{cases}$$

therefore

$$|y_i| = \min\{|x_i^* - m_1|, |x_i^* - m_2|\} \tag{15}$$

holds for $i = 1, \ldots, n$. Denote

$$\sigma^2(\mathbf{y}) = \sum_{i=1}^{n} d_i y_i^2$$

the variance of the coordinates of $\mathbf{y}$. Since, due to (15), the weighted 2-variance of the coordinates of $\mathbf{x}^*$ is one of the terms behind the minimum in (9), $\sigma^2(\mathbf{y}) \geq s^2$. In the case of $\sigma(\mathbf{y}) = 0$, the 2-variance s^2 is also equal to 0, and the statement of the theorem is automatically true (but this cannot occur if 0 is a single eigenvalue of $\boldsymbol{L}_D$). Therefore, $\sigma(\mathbf{y}) > 0$ can be assumed. Define the vector $\mathbf{z} \in \mathbb{R}^n$ of the following coordinates:

$$z_i = \frac{y_i}{\sigma(y)}, \quad i = 1, \ldots, n$$

and let $\mathbf{x}_i = (x_i^*, z_i)$ be 2-dimensional vector, a possible representative of vertex i. Further, let

$$\boldsymbol{X} = (\mathbf{x}^*, \mathbf{z}) \quad \textit{and} \quad \boldsymbol{X}^* = (\mathbf{x}^*, \boldsymbol{D}^{-1/2}\mathbf{u}_3)$$

be $n \times 2$ matrices, where $\boldsymbol{X}$ contains the representatives $\mathbf{x}_i$'s, while $\boldsymbol{X}^*$ contains the optimal 2-dimensional representatives in its rows. (In fact, they are 3-dimensional representatives, but we disregard the first, constantly 1, coordinates.) Then, on the one hand,

$$\max_{x_i^* \neq x_j^*} \frac{|z_i - z_j|}{|x_i^* - x_j^*|} \leq \frac{1}{\sigma(\mathbf{y})},$$

since due to the definition of y_i, the relation

$$|y_i - y_j| \leq |x_i^* - x_j^*| \quad (i \neq j)$$

holds, i.e. y_i's (as functions of x_i^*'s) satisfy the Lipschitz condition (with constant 1).

On the other hand,

$$\frac{\lambda_1+\lambda_2}{\lambda_1} = \frac{\mathrm{tr}(\boldsymbol{X}^{*T}\boldsymbol{L}\boldsymbol{X}^*)}{\mathbf{x}^{*T}\boldsymbol{L}\mathbf{x}^*} \le \frac{\mathrm{tr}(\boldsymbol{X}^{T}\boldsymbol{L}\boldsymbol{X})}{\mathbf{x}^{*T}\boldsymbol{L}\mathbf{x}^*} = \frac{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\|\mathbf{x}_i-\mathbf{x}_j\|^2}{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}(x_i^*-x_j^*)^2}$$
$$= \frac{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}\left[\,(x_i^*-x_j^*))^2+(z_i-z_j)^2\,\right]}{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} w_{ij}(x_i^*-x_j^*)^2}$$
$$\le 1+\max_{x_i^*\neq x_j^*}\frac{(z_i-z_j)^2}{(x_i^*-x_j^*)^2} \le 1+\frac{1}{\sigma^2(\mathbf{y})} \le 1+\frac{1}{s^2},$$

which – by subtracting 1 from both the left- and right-hand sides and taking the reciprocals – finishes the proof.

Theorem 2 indicates the following two-clustering property of the two smallest positive normalized Laplacian eigenvalues: the greater the gap between them, the better the optimal 2-dimensional (if fact, one-dimensional) representatives of the vertices can be classified into two clusters. This fact, via Theorem 1 implies that the gap between the eigenvalues λ_1 and λ_2 of $\boldsymbol{L}_D$ is sufficient for the graph to have a small 2-way normalized cut. For $k > 2$, the situation is more complicated, as will be discussed in the next section.

2 The isoperimetric number and sparse cuts

For the two-cluster case, the normalized cut of Section 1 is the symmetric version of the isoperimetric number (sometimes called Cheeger constant) introduced in the context of Riemannian manifolds (see e.g. [22]) and much earlier, in mathematical physics. There is a wide literature of this topic together with expander graphs, see e.g. [4, 21, 26, 39, 52, 55, 56] and [23], for a summary. We just discuss the most important relations of this topic to sparse, balanced cuts and clustering.

Definition 2 *Let $G = (V, \boldsymbol{W})$ be an edge-weighted graph with generalized degrees $d_1, \ldots, d_n$ and assume that $\sum_{i=1}^n d_i = 1$. The isoperimetric number of G is*

$$h(G) = \min_{\substack{U\subset V\\ \mathrm{Vol}(U)\le\frac{1}{2}}} \frac{w(U,\overline{U})}{\mathrm{Vol}(U)}. \tag{16}$$

Since $\mathrm{Vol}(U)$ is the sum of the weights of edges emanating from U, while $w(U,\overline{U})$ is sum of the weights of those connecting U and $\overline{U}$, the relation $0 \le h(G) \le 1$ is trivial. Further, $h(G) = 0$ if and only if G is disconnected; therefore, only isoperimetric number of a connected graph is of interest. The isoperimetric number will later be considered as conditional probability, but first we investigate its relation to the smallest positive normalized Laplacian eigenvalue. Note that for simple graphs, $h(G)$ is not identical to the combinatorial isoperimetric number $i(G)$ which uses the cardinality of the subsets instead of their volumes in the denominator of (16), and hence, can exceed 1, see [56] for details. More precisely, the combinatorial isoperimetric number of the simple graph G is defined

by

$$i(G) = \min_{\substack{S\subset V \\ 0<|S|\leq \frac{n}{2}}} \frac{e(S,\overline{S})}{|S|}.$$

It is sometimes called edge-expansion, and mainly used for regular graphs, see [39]. The authors of the aforementioned paper also note that a graph is a 'good' expander if it is simultaneously sparse and highly connected.

Intuitively, $h(G)$ is 'small' if 'few low-weight' edges connect together two disjoint vertex-subsets (forming a partition of the vertices) with 'not significantly' differing volumes; therefore, a 'small' $h(G)$ is an indication for a sparse cut of G. On the contrary, a 'large' $h(G)$ means that any vertex-subset of G has a large boundary compared to its volume, where the boundary of $U \subset V$ is the weighted cut between U and its complement in V. This is called good edge-expanding property of G, but we do not want to give the exact definition of an expander graph which depends on many parameters and discussed in details (distinguishing between edge- and vertex-expansion) in many other places, see e.g. [3, 5, 39, 52].

Now, a two-sided relation between $h(G)$ and the normalized Laplacian eigenvalue λ_1 is stated for edge-weighted graphs in the following theorem. Similar statements are proved in [23, 56, 4] for simple graphs and in [69] for edge-weighted graphs, but without the upcoming improved upper bound.

Theorem 3 (Cheeger inequality) *Let $G = (V, \boldsymbol{W})$ be a connected edge-weighted graph with isoperimetric number $h(G)$, and let λ_1 denote the smallest positive eigenvalue of its normalized Laplacian $\boldsymbol{L}_D$. Then*

$$\frac{\lambda_1}{2} \leq h(G) \leq \min\{1, \sqrt{2\lambda_1}\}$$

always holds true. Furthermore, provided $\lambda_1 \leq 1$, the upper estimate improves to

$$h(G) \leq \sqrt{\lambda_1(2-\lambda_1)}.$$

Note that $\lambda_1 \leq 1$ is not a peculiar requirement as, by Remark **??** (iv), except the complete graph, every simple graph satisfies this requirement.

We will follow the proof of [17].

Proof 3

- *Lower bound. It follows from the lower estimate (3) of the normalized cut (see Theorem 1). Indeed, in the $k = 2$ case, this gives $\lambda_1 \leq f_2(G)$. By the definition of the normalized cut,*

$$f_2(G) = \min_{(U,\overline{U})} \frac{w(U,\overline{U})}{\mathrm{Vol}(U)\mathrm{Vol}(\overline{U})} \leq 2 \min_{\mathrm{Vol}(U)\leq\frac{1}{2}} \frac{w(U,\overline{U})}{\mathrm{Vol}(U)} = 2h(G),$$

  where we used that $\mathrm{Vol}(U) + \mathrm{Vol}(\overline{U}) = 1$, and because of the symmetry, assuming $\mathrm{Vol}(U) \leq \frac{1}{2}$ and $\mathrm{Vol}(\overline{U}) \geq \frac{1}{2}$ is not a restriction. These facts together imply that $\lambda_1 \leq 2h(G)$ which provides the required lower bound.

- *Upper bound. We will follow the proof of [17].*

  With the notation of Section 1, let $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1} \leq 2$ be the spectrum of $\boldsymbol{L}_D$ and $\mathbf{u}_1$ be unit-norm eigenvector corresponding to λ_1. Let

$\mathbf{x}^* = \boldsymbol{D}^{-1/2}\mathbf{u}_1$ *contain the optimal representatives of the vertices in its coordinates (we omit the trivial dimension) for which* $\sum_{i=1}^n d_i x_i^* = 0$ *and* $\sum_{i=1}^n d_i x_i^{*2} = 1$ *holds, see also (10) in the proof of Theorem 2. Without loss of generality,* $\mathbf{x}^*$ *is directed such that*

$$\sum_{i:\, x_i^*<0} d_i \geq \sum_{i:\, x_i^*\geq 0} d_i.$$

From now on, the superscript of $\mathbf{x}^*$ *is discarded for notational convenience. We rearrange the coordinates of* $\mathbf{x}$ *in increasing order:*

$$x_1 \leq \cdots \leq x_{r-1} < 0 \leq x_r \leq \cdots \leq x_n.$$

Actually, we took advantage of the fact that there are both negative and positive numbers among the coordinates of $\mathbf{x}$*, because of the relation* $\sum_{i=1}^n d_i x_i = 0$*. Say, the number of strictly negative coordinates is* $r-1$*,* $r \geq 2$*. The vertex set* $V = \{1, \ldots, n\}$ *is rearranged, accordingly. Put* $V_- := \{1, \ldots, r-1\}$ *and* $V_+ := \{r, \ldots, n\}$*.*

By the above assumption, for the coordinates of $\mathbf{x}$ *we have that*

$$\sum_{i=1}^{r-1} d_i \geq \sum_{i=r}^{n} d_i. \tag{17}$$

Set $\mathbf{y} := \mathbf{x}_+$*, that is the coordinates of the vector* $\mathbf{y}$ *are*

$$y_i = \begin{cases} x_i & \text{if} \quad x_i \geq 0 \\ 0 & \text{if} \quad x_i < 0. \end{cases}$$

We will choose special two-partitions of the rearranged vertex-set induced by the subsets $U_k = \{k, \ldots, n\}$ *and put*

$$c_k = w(U_k, \overline{U_k}) \quad (k = 2, \ldots, n). \tag{18}$$

Obviously,

$$h(G) \leq c = \min_{2\leq k\leq n} \frac{c_k}{\min\{\mathrm{Vol}(U_k), \mathrm{Vol}(\overline{U_k})\}}. \tag{19}$$

We remark that in view of (17), the relation

$$\min\{\mathrm{Vol}(U_k), \mathrm{Vol}(\overline{U_k})\} = \mathrm{Vol}(U_k) = \sum_{i=k}^{n} d_i \quad \text{for} \quad k = r, \ldots, n \tag{20}$$

is valid.

As $\boldsymbol{D}^{1/2}\mathbf{x}$ *is an eigenvector of* $\boldsymbol{L}_D = \boldsymbol{I}_n - \boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$ *with eigenvalue* λ_1*,*

$$\lambda_1 \boldsymbol{D}\mathbf{x} = \boldsymbol{D}\mathbf{x} - \boldsymbol{W}\mathbf{x},$$

or equivalently, for the coordinates,

$$\lambda_1 d_i x_i = d_i x_i - \sum_{j=1}^{n} w_{ij} x_j = \sum_{j=1}^{n} w_{ij}(x_i - x_j), \quad i = 1 \ldots, n \tag{21}$$

holds.

Multiplying both sides of (21) by x_i and summing for indices $i \in V_+$, we get that

$$\lambda_1 \sum_{i \in V_+} d_i x_i^2 = \sum_{i \in V_+} x_i \sum_{j=1}^{n} w_{ij}(x_i - x_j),$$

or equivalently,

$$\lambda_1 = \frac{\sum_{i \in V_+} x_i \sum_{j=1}^{n} w_{ij}(x_i - x_j)}{\sum_{i \in V_+} d_i x_i^2} =: \frac{A}{\sum_{i=1}^{n} d_i y_i^2}. \tag{22}$$

Now, we will estimate the numerator (A) from below as follows:

$$\begin{aligned}
A &= \sum_{i \in V_+} \sum_{j \in V_+} w_{ij} x_i (x_i - x_j) + \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} x_i (x_i - x_j) \\
&= \sum_{\substack{i \in V_+,\, j \in V_+ \\ i > j}} [w_{ij} x_i (x_i - x_j) + w_{ji} x_j (x_j - x_i)] + \\
&+ \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} x_i^2 - \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} x_i x_j \\
&\overset{(1)}{=} \sum_{\substack{i \in V_+,\, j \in V_+ \\ i > j}} w_{ij} (x_i - x_j)^2 + \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} y_i^2 - \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} x_i x_j \\
&\overset{(2)}{\geq} \sum_{\substack{i \in V_+,\, j \in V_+ \\ i > j}} w_{ij} (y_i - y_j)^2 + \sum_{i \in V_+} \sum_{j \in V_-} w_{ij} (y_i - y_j)^2 \\
&\overset{(3)}{=} \sum_{i \in V_+} \sum_{j < i} w_{ij} (y_i - y_j)^2 = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (y_i - y_j)^2.
\end{aligned}$$

In the steps (1) and (2) we used the fact that y_i is equal to x_i on V_+ and 0 on V_-. We decreased the expression between the two steps by $-\sum_{i \in V_+} \sum_{j \in V_-} w_{ij} x_i x_j$ that is a nonnegative quantity due to the different signs of x_i and x_j for indices $i \in V_+$ and $j \in V_-$. In the step (3) we utilized that for such indices $i > j$ automatically holds true. We also used the symmetry of $\boldsymbol{W}$ several times.

Now, let us go back to (22). Using the lower estimate for A we get that

$$\lambda_1 \geq \frac{\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} (y_i - y_j)^2}{\sum_{i=1}^{n} d_i y_i^2} =: Q. \tag{23}$$

The quantity Q defined above will be important later when we improve the

estimate. Q will be further decreased as follows.

$$
\begin{aligned}
Q &= \frac{\frac{1}{2}\left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i - y_j)^2\right] \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]} \\
&= \frac{1}{2}\frac{\left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}|y_i - y_j|^2\right] \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}|y_i + y_j|^2\right]}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]} \\
&\geq \frac{1}{2}\frac{\left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}|y_i - y_j| \cdot |y_i + y_j|\right]^2}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]} \\
&= \frac{1}{2}\frac{\left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}|y_i^2 - y_j^2|\right]^2}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]^2} \\
&= \frac{1}{2}\frac{\left[2\sum_{i>j} w_{ij}|y_i^2 - y_j^2|\right]^2}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]} \\
&= 2\frac{\left[\sum_{i>j} w_{ij}(y_i^2 - y_j^2)\right]^2}{\sum_{i=1}^n d_i y_i^2 \cdot \left[\sum_{i=1}^n \sum_{j=1}^n w_{ij}(y_i + y_j)^2\right]} =: 2\frac{A_1^2}{B}.
\end{aligned}
\tag{24}
$$

In the third line we used the Cauchy–Schwarz inequality for the expectation of the random variables $|Y - Y'|$ and $|Y + Y'|$ with the symmetric joint distribution given by $\boldsymbol{W}$, where Y and Y' are identically distributed according to the marginal degree distribution and taking on values y_i's.

To estimate A_1 from below, we will use the fact that $y_i \geq y_j$ for $i > j$ and write the terms $y_i^2 - y_j^2$ as a telescopic sum:

$$y_i^2 - y_j^2 = (y_i^2 - y_{i-1}^2) + \cdots + (y_{j+1}^2 - y_j^2) \quad \textit{for} \quad i > j.$$

By this,

$$
\begin{aligned}
A_1 &= \sum_{i>j} w_{ij}(y_i^2 - y_j^2) = \sum_{k=2}^n (y_k^2 - y_{k-1}^2) \sum_{i \geq k > j} w_{ij} \overset{(4)}{=} \sum_{k=2}^n (y_k^2 - y_{k-1}^2) c_k \\
&= \sum_{k=r}^n (y_k^2 - y_{k-1}^2) c_k \overset{(5)}{\geq} \sum_{k=r}^n (y_k^2 - y_{k-1}^2) c \sum_{i=k}^n d_i \geq \sum_{k=r}^n (y_k^2 - y_{k-1}^2) h \sum_{i=k}^n d_i \\
&= h(G) \sum_{k=r}^n (y_k^2 - y_{k-1}^2) \sum_{i=k}^n d_i \overset{(6)}{=} h \sum_{k=r}^n y_k^2 d_k
\end{aligned}
$$

where in (4) we used the definition of c_k, in (5) the relations (19) and (20) were exploited, while in (6) a partial summation was performed.

The denominator B is estimated from above as follows:

$$B=\sum_{i=1}^{n} d_i y_i^2\left[\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(y_i+y_j)^2\right] \le \sum_{i=1}^{n} d_i y_i^2\left[\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(2y_i^2+2y_j^2)\right]$$
$$=\sum_{i=1}^{n} d_i y_i^2\left[4\sum_{i=1}^{n} y_i^2 d_i\right]=4\left(\sum_{i=1}^{n} y_i^2 d_i\right)^2.$$

There remains to collect the terms together:

$$\lambda_1 \ge \frac{2A_1^2}{B} \ge \frac{2h^2(G)\left(\sum_{k=1}^{n} y_k^2 d_k\right)^2}{4\left(\sum_{i=1}^{n} y_i^2 d_i\right)^2}=\frac{h^2(G)}{2},$$

and hence, the upper estimate $h(G)\le\sqrt{2\lambda_1}$ follows.

We can improve this upper bound by using the exact value of B and going back to (23) that implies

$$\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(y_i-y_j)^2=2Q\sum_{i=1}^{n} d_i y_i^2.$$

An equivalent form of B is

$$B=\sum_{i=1}^{n} d_i y_i^2\cdot\left[\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(y_i+y_j)^2\right]=\sum_{i=1}^{n} d_i y_i^2\left[\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(2y_i^2+2y_j^2-(y_i-y_j)^2)\right]$$
$$=\sum_{i=1}^{n} d_i y_i^2\left[4\sum_{i=1}^{n} y_i^2 d_i-\sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}(y_i-y_j)^2\right]=2\left(\sum_{i=1}^{n} d_i y_i^2\right)^2(2-Q).$$

Starting the estimation of Q at (24) and continuing with the B above, yields

$$Q\ge 2\frac{A_1^2}{B}\ge 2\frac{h^2(\sum_{k=1}^{n} y_k^2 d_k)^2}{2(\sum_{i=1}^{n} d_i y_i^2)^2(2-Q)}=\frac{h^2(G)}{2-Q}.$$

In view of (23), Q is nonnegative, implying

$$Q\ge\frac{h^2}{2-Q}\quad \textit{or equivalently,}\quad 1-\sqrt{1-h^2(G)}\le Q\le 1+\sqrt{1-h^2(G)}.$$

Summarizing, we derive that

$$\lambda_1\ge Q\ge 1-\sqrt{1-h^2(G)}\quad \textit{or equivalently,}\quad \sqrt{1-h^2(G)}\ge 1-\lambda_1.$$

For $\lambda_1>1$ this is a trivial statement. For $\lambda_1<1$ it implies that $h(G)\le\sqrt{\lambda_1(2-\lambda_1)}<1$, while for $\lambda_1=1$ we get the trivial bound $h(G)\le 1$. This finishes the proof.

In the framework of joint distributions, $h(G)$ can be viewed as a conditional probability and related to the symmetric maximal correlation in the following way. The weight matrix $\boldsymbol{W}$ (with sum of its entries 1) defines a discrete symmetric joint distribution $\mathbb{W}$ with equal marginals $\mathbb{D}=\{d_1,\dots,d_n\}$. Let H denote

the Hilbert space of $V \to \mathbb{R}$ random variables taking on at most n different values with probabilities $d_1, \ldots, d_n$, and having zero expectation and finite variance. Let us take two identically distributed (i.d.) copies $\psi, \psi' \in H$ with joint distribution $\mathbb{W}$. Then, obviously,

$$h(G) = \min_{\substack{B \subset \mathbb{R} \text{ Borel-set} \\ \psi, \psi' \in H \text{ i.d.} \\ \mathbb{P}_{\mathbb{D}}(\psi \in B) \leq 1/2}} \mathbb{P}_{\mathbb{W}}(\psi' \in \overline{B} | \psi \in B).$$

The symmetric maximal correlation defined by the symmetric joint distribution $\mathbb{W}$ is the following:

$$r_1 = \max_{\psi, \psi' \in H \text{ i.d.}} \mathrm{Corr}_{\mathbb{W}}(\psi, \psi') = \max_{\substack{\psi, \psi' \in H \text{ i.d.} \\ \mathrm{Var}_{\mathbb{D}} \psi = 1}} \mathrm{Cov}_{\mathbb{W}}(\psi, \psi').$$

Then $r_1 = 1 - \lambda_1$, provided $\lambda_1 \leq 1$.

With this notation, the result of Theorem 3 can be written in the equivalent form as follows.

Proposition 1 *Let $\mathbb{W}$ be the symmetric joint distribution of two discrete random variables taking on at most n different values, where the joint probabilities of $\mathbb{W}$ are the entries of the weight matrix $\boldsymbol{W}$. If the symmetric maximal correlation r_1 is nonnegative, then with it, the estimation*

$$\frac{1 - r_1}{2} \leq \min_{\substack{B \subset \mathbb{R} \, Borel\text{-}set \\ \psi, \psi' H \, i.d. \\ \mathbb{P}_{\mathbb{D}}(\psi \in B) \leq 1/2}} \mathbb{P}_{\mathbb{W}}(\psi' \in \overline{B} | \psi \in B) \leq \sqrt{1 - r_1^2}$$

holds.

Proof 4 *Since $\lambda_1 = 1 - r_1$, the lower bound trivially follows. $r_1 \geq 0$ implies that $\lambda_1 \leq 1$, so the improved upper bound of Theorem 3 becomes $\sqrt{(1 - r_1)(1 + r_1)}$ which finishes the proof.*

Consequently, the symmetric maximal correlation somehow regulates the minimum conditional probability that provided a random variable takes values in a category set (with probability less than $1/2$) then another copy of it (their joint distribution is given by $\boldsymbol{W}$) will take values in the complementary category set. The larger r_1, the smaller this minimum conditional probability is. In particular, if r_1 is the largest absolute value eigenvalue of $\boldsymbol{I} - \boldsymbol{L}_D$ (apart from the trivial 1), then r_1 is the usual maximal correlation.

The other important application of the isoperimetric inequality is related in many aspects to random walks. We just touch upon to this topic here, for the interested readers we refer to [2, 10, 26, 23, 49, 50, 51, 74, 70].

In fact, time-reversible Markov chains can be viewed as random walks on undirected, possibly edge-weighted graphs ($\boldsymbol{W}$ is symmetric). The walk can be described by a discrete time stochastic process $\xi_0, \xi_1, \ldots, \xi_t, \ldots$ with finite state space $\{1, \ldots, n\}$. The transition probabilities

$$\mathbb{P}(\xi_{t+1} = j \,|\, \xi_t = i) = \frac{w_{ij}}{d_i}$$

do not depend on t and are entries of the *transition probability matrix* $\boldsymbol{D}^{-1}\boldsymbol{W}$. The transition probability matrix is not symmetric, but its spectrum is the

same as that of the symmetric matrix $\boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$, since the eigenvalue–eigenvector equation

$$\boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}\mathbf{u} = \lambda\mathbf{u}$$

is equivalent to

$$\boldsymbol{D}^{-1}\boldsymbol{W}(\boldsymbol{D}^{-1/2}\mathbf{u}) = \lambda(\boldsymbol{D}^{-1/2}\mathbf{u}).$$

Therefore, the transition probability matrix has real eigenvalues in the $[-1, 1]$ interval, they are the numbers $1 - \lambda_i$, where λ_i is the ith largest eigenvalue of $\boldsymbol{L}_D$, and corresponding eigenvectors which are the vector components of the optimal representation. Further, its largest eigenvalue is always 1 with corresponding eigendirection $\mathbf{1}$, and the multiplicity of 1 as an eigenvalue is equal to the number of the connected components of G. The random walk is ergodic if it has a unique stationary distribution. The necessary and sufficient condition of ergodicity is the irreducibility ($\lambda_1 > 0$) and aperiodicity ($\lambda_{n-1} < 2$). Therefore a random walk on a connected and non-bipartite graph exhibits a unique stationary distribution which is just $\{d_1, \ldots, d_n\}$. The so-called *mixing rate* shows how rapidly the random walk converges to this stationary distribution. By the Cheeger inequality (Theorem 3) it follows that a relatively large λ_1 induces rapid mixing and short *cover time* which is the expected number of time to reach every vertex (starting from a given distribution), see [49]. The electric network analogue, including *conductance* of random walks on graphs is discussed thoroughly e.g. by [70, 71, 72].

We are rather interested in the case when λ_1 is near zero and the random walk cannot go through quickly the graph because of bottlenecks in it. Such a bottleneck can be the weighted cut between two disjoint and mutually exhaustive vertex-subsets which give the minimum in the definition of $h(G)$. More generally, if there are $k - 1$ near zero eigenvalues of $\boldsymbol{L}_D$, then we may expect k clusters such that the random walk stays with high probability within the clusters and goes through between the cluster pairs ($\binom{k}{2}$ bottlenecks) with smaller probability. This assumption is formulated by the normalized cuts (introduced in Definition 1) and sparse cuts, to be introduced.

Note that because of the relation $f_2(G) \leq 2h(G)$ (we saw this when proved the lower bound in the Cheeger inequality), Theorem 3 and Theorem 1 provide us with the following estimation of the 2-way normalized cut of G with the help of its smallest positive normalized Laplacian eigenvalue, in the $\lambda_1 \leq 1$ typical case:

$$\lambda_1 \leq f_2(G) \leq 2\sqrt{\lambda_1(2 - \lambda_1)}.$$

There are several natural generalizations of the isoperimetric number for $k > 2$ and of the Cheeger inequality for the upper end of the normalized Laplacian spectrum. We will discuss some recent results that directly relate so-called k-way sparse cuts to the eigenvalue λ_{k-1}.

In [73], the so-called dual Cheeger inequality is proved which estimates the measure $\beta(G)$ of bipartiteness of G by means of the upper spectral gap of $\boldsymbol{L}_D$, i.e. the difference between λ_{n-1} and 2. To be consistent with the previous notation, $0 = \lambda_0 \leq \cdots \leq \lambda_{n-1} \leq 2$ will stand for the normalized Laplacian spectrum.

Definition 3 *The bipartiteness ratio of the simple, d-regular graph G on the*

n-element vertex set V is

$$\beta(G) = \min_{\substack{S \subset V \\ (L,R)\ 2\text{-partition of } S}} \frac{2e(L) + 2e(R) + e(S, \overline{S})}{d|S|}$$

where $e(L)$ and $e(R)$ stands for the number of edges between vertices of L and R, respectively, and $e(S, \overline{S})$ denotes the number of cut-edges.

Note that the left and right non-empty, disjoint subsets of S ($L \cup R = S$) not necessarily exhaust V. Since there are no loops, $e(L, L) = 2e(L)$ and $e(R, R) = 2e(R)$.

Proposition 2 (Dual Cheeger inequality)

$$\frac{1}{2}(2 - \lambda_{n-1}) \leq \beta(G) \leq \sqrt{2(2 - \lambda_{n-1})}$$

where λ_{n-1} is the largest eigenvalue of the normalized Laplacian $\boldsymbol{L}_D$.

Note that the original paper uses the eigenvalues of the matrix $\boldsymbol{D}^{-1/2}\boldsymbol{W}\boldsymbol{D}^{-1/2}$, especially, $|1 - \lambda_{n-1}|$ in the formulation of the dual Cheeger inequality. Observe that $\lambda_{n-1} \geq \frac{n}{n-1} \geq 1$, therefore $1 - \lambda_{n-1} < 0$ always holds.

Observe that if G is bipartite, then $\lambda_{n-1} = 2$ and $\beta(G) = 0$. The proposition implies that $\beta(G)$ is small if λ_{n-1} is close to 2, i.e. a large λ_{n-1} is an indication for G having a closely bipartite induced subgraph that is relatively large and sparsely connected to the other part of G.

We also remark that the notion of the bipartiteness ratio can naturally be extended to an edge-weighted graph $G = (V, \boldsymbol{W})$ in the following way:

$$\beta(G) = \min_{\substack{S \subset V \\ (L,R)\ 2\text{-partition of } S}} \frac{w(L, L) + w(R, R) + w(S, \overline{S})}{\mathrm{Vol}(S)}.$$

Probably, a similar estimation with it for the upper spectral gap of an edge-weighted graph exists. Analogously to Theorem 2, in [19] the upper spectral gap was used to estimate the 2-variance of the 1-dimensional vertex representatives, based on the coordinates of the vector $\boldsymbol{D}^{-1/2}\mathbf{u}_{n-1}$. The relation between bipartite subgraphs and the smallest adjacency eigenvalue (corresponding to the largest normalized Laplacian one if the graph is regular) is also treated in [6].

Now we discuss some recent results of [45, 46, 47] on possible extensions of the Cheeger inequality to multiway cuts, called *higher-order Cheeger inequalities*. For the edge-weighted graph $G = (V, \boldsymbol{W})$, the *expansion* of the vertex-subset $S \subseteq V$ is defined by

$$\phi(S, G) = \frac{w(S, \overline{S})}{\mathrm{Vol}(S)}. \tag{25}$$

Note that in [45] it is formulated for simple, d-regular graphs with $e(S, \overline{S})$ in the numerator and $d|S|$ in the denominator. In [47], the authors define this expansion for edge-weighted graphs, but use $\min\{\mathrm{Vol}(S), \mathrm{Vol}(\overline{S})\}$ in the denominator. However, this does not make any difference in the upcoming definition.

Definition 4 *For a given integer $1 < k < n$, the k-way expansion constant of the edge weighted graph $G = (V, \boldsymbol{W})$ on n vertices is*

$$\rho_k(G) = \min_{\substack{S_1,\ldots,S_k \subset V \\ S_i \neq \emptyset,\, i,\ldots,k \\ S_i \cap S_j = \emptyset,\, i \neq j}} \max_{i \in \{1,\ldots,k\}} \phi(S_i, G).$$

Note that here the collection of pairwise disjoint subsets $S_1, \ldots, S_k$ is not necessarily a k-partition, since the do not always exhaust V.

It is easy to see that $\rho_2(G) = h(G)$ and therefore, the Cheeger inequality bounds it from below and from above in terms of λ_1. In [45] a similar relation is proved for $\rho_k(G)$, for a general k, in terms of the kth smallest normalized Laplacian eigenvalue λ_{k-1}. We cite this result with our notation.

Theorem 4

$$\frac{\lambda_{k-1}}{2} \leq \rho_k(G) \leq \mathcal{O}(k^2)\sqrt{\lambda_{k-1}}.$$

With fewer sets than the order of the eigenvalue, the upper estimate improves to

$$\rho_k(G) \leq \mathcal{O}(\sqrt{\lambda_{2k-1} \log k}). \tag{26}$$

The proof of Theorem 4 is algorithmic. It uses the optimum k-dimensional representatives of the vertices and applies geometric considerations to them. Namely, it is shown that the total mass of them is localized on k disjoint regions of $\mathbb{R}^k$ (in fact, in a $(k-1)$-dimensional hyperplane of it). Observe that this notion is closely related to our weighted k-variance introduced in Lesson 1. Otherwise, to find these sparsest cuts is NP-complete.

Both in [45] and [47] a sparsest small set, producing some kind of sparse cut of G and comprising at most the $1/k$ fraction of the total volume, is defined as follows with our notation.

Definition 5 *For a given integer $1 < k < n$, the small-set sparsity of the edge weighted graph $G = (V, \boldsymbol{W})$ on n vertices is defined by*

$$\phi_k(G) = \min_{\substack{S \subset V \\ \mathrm{Vol}(S) \leq \mathrm{Vol}(V)/k}} \phi(S, G).$$

Obviously, $\phi_k(G) \leq \rho_k(G)$, for every positive integer $k < n$. Therefore, Inequality (26) implies that

$$\phi_{k/2}(G) \leq \mathcal{O}(\sqrt{\lambda_{k-1} \log k})$$

which improves a statement of [46] that

$$\phi_{\sqrt{k}}(G) \leq C(\sqrt{\lambda_{k-1} \log k}),$$

where C is a fixed constant.

We remark that the small set problem is closely related to Unique Games. In this context, [8] showed that $\phi_k(G) < C\sqrt{\lambda_{(k-1)^{100}} \log_k n}$, where C is some absolute constant.

To find the sparsest k-partition, in [46] an iterative algorithm is defined which finds the sparsest 2-way cut in each step and removes the cut-edges. Meanwhile,

the graph becomes disconnected, and the algorithm operates on the components of it. The authors also prove that for any edge-weighted graph $G = (V, \boldsymbol{W})$ and any integer $1 \leq k \leq |V|$, there exist ck disjoint subsets $S_1, \ldots, S_{ck}$ of V such that

$$\max_i \phi(S_i, G) \leq C\sqrt{\lambda_{k-1} \log k}$$

where $c < 1$ and C are absolute constants. Moreover, these sets can be identified in polynomial time. In [45], the authors find a so-called non-expanding k-partition $V_1, \ldots, V_k$ of V such that

$$\phi(V_i, G) \lesssim k^4\sqrt{\lambda_{k-1}}, \quad i = 1, \ldots, k.$$

We remark that between the k-way expansion constant and the normalized cut the following relation holds:

$$\rho_k(G) \leq \min_{(V_1,\ldots,V_k)=P_k} \max_{i\in\{1,\ldots,k\}} \phi(V_i, G) \leq \min_{(V_1,\ldots,V_k)=P_k} \sum_{i=1}^{k} \phi(V_i, G) = f_k(G)$$

where we took into consideration the equivalent forms (1) of the normalized cut. If the minimum in $\rho_k(G)$ is attained at a k-partition, then

$$f_k(G) = \min_{(V_1,\ldots,V_k)=P_k} \sum_{i=1}^{k} \phi(V_i, G) \leq k \min_{(V_1,\ldots,V_k)=P_k} \max_{i\in\{1,\ldots,k\}} \phi(V_i, G) = k\rho_k(G).$$

In this case, Theorem 4 also implies $f_k(G) \leq \mathcal{O}(k^3)\sqrt{\lambda_{k-1}}$.

Consequently, there are the k-way sparsest cuts which are closely related to λ_{k-1}. However, a small λ_{k-1} is not always an indication of a small normalized cut. In fact, λ_{k-1} can be small if there exist a sparse system $S_1, \ldots, S_k$ which not necessarily exhaust V. The other parts of V may have, for example, closely bipartite subgraphs, etc. When later we define so-called regular cuts, we will illustrate that there are the small and large normalized Laplacian eigenvalues which together recover the graph's structure, and regular cuts may contain sparse and dense cuts as well.

3 The Newman–Girvan modularity

The Newman–Girvan modularity introduced in [58] directly focuses on modules of higher intra-community connections than expected based on the model of independent attachment of the vertices with probabilities proportional to their degrees. To maximize this modularity, hierarchical clustering methods based on the edge betweenness measure of [58, 59, 60, 24], and vector partitioning algorithms based on the eigenvectors of the modularity matrix of [62] are introduced. In [29] an extremal optimization algorithm is presented.

We will extend the linear algebraic machinery developed for Laplacian based spectral clustering to the modularity based community detection. To this end, two penalized versions of the Newman–Girvan modularity are introduced in the general framework of an edge-weighted graph, see [61], and their relation to projections onto the subspace of partition vectors and to k-variance of the clusters formed by the vertex representatives is investigated. These considerations give useful information on the choice of k and on the nature of the community structure.

Definition 6 *The Newman-Girvan modularity corresponding to the k-partition $P_k = (V_1, \ldots, V_k)$ of the vertex-set of the edge-weighted graph $G = (V, \boldsymbol{W})$, where the entries of $\boldsymbol{W}$ sum to 1, is*

$$M(P_k, G) = \sum_{a=1}^{k} \sum_{i,j \in V_a} (w_{ij} - d_i d_j) = \sum_{a=1}^{k} [w(V_a, V_a) - \mathrm{Vol}^2(V_a)].$$

For given integer $1 \leq k \leq n$, the k-module Newman-Girvan modularity of the edge-weighted graph G is

$$M_k(G) = \max_{P_k \in \mathcal{P}_k} M(P_k, G).$$

For a simple graph, $w(V_a, V_a) = 2e(V_a)$ is twice the number of edges with both endpoints in in V_a, and $\mathrm{Vol}(V_a)$ is the number of edges emanating from V_a. The entries $d_i d_j$ of the null-model matrix $\mathbf{d}\mathbf{d}^T$ correspond to the hypothesis of independence. In other words, under the null-hypothesis, vertices i and j are connected to each other independently, with probability $d_i d_j$ proportional (actually, because the sum of the weights is 1, equal) to their generalized degrees $(i, j = 1, \ldots, n)$. Hence, for given k, maximizing $M(P_k, G)$ is equivalent to looking for k modules of the vertices with intra-community connections higher than expected under the null-hypothesis. As $\sum_{a=1}^{k} \sum_{b=1}^{k} \sum_{i \in V_a} \sum_{j \in V_b} (w_{ij} - d_i d_j) = 0$, the above task is equivalent to minimizing

$$\sum_{a \neq b} \sum_{i \in V_a,\, j \in V_b} (w_{ij} - d_i d_j), \tag{27}$$

that is, to looking for k clusters of the vertices with inter-cluster connections lower than expected under the hypothesis of independence. In the minimum cut problem the cumulated inter-cluster connections themselves were minimized. Therefore, the spectral method introduced in [75] for maximizing the Newman-Girvan modularity is closely related to that of [54, 64, 13] for minimizing the normalized cut.

We want to penalize partitions with clusters of extremely different sizes. To measure the size of cluster V_a, either the number of its vertices $|V_a|$ or its volume $\mathrm{Vol}(V_a)$ is used. [34] remarks that the Newman–Girvan modularity seems to attain its maximum for clusters of near equal sizes, though there is no explanation for it. Of course, communities of real-life networks have more practical relevance if they do not differ too much in sizes. In [59] and [67], the authors also define a good modularity structure as one having near equal sizes of modules. However, they do not make use of this idea in their objective function. Actually, [67] prove that the Newman–Girvan modularity is a special ground state energy, the convergence of the ground state energies is used to prove the testability of some balanced multiway cut densities. However, these conditional extrema cannot be immediately related to spectra. As a compromise, we modify the modularity itself so that it would penalize clusters of significantly different sizes. Of course, real-life communities are sometimes very different in sizes or volumes. Our method is capable to find fundamental clusters, and further analysis is needed to separate small communities from the large ones. Other possibility is to distinguish a core of the graph that is free of low-degree vertices for which, usually near zero eigenvalues are responsible.

As in the case of $k > 2$, there are more inter-cluster sums than intra-cluster ones, it is in (27), where we penalize clusters of too different sizes or volumes by introducing a factor $\frac{1}{|V_a|} + \frac{1}{|V_b|}$ or $\frac{1}{\mathrm{Vol}(V_a)} + \frac{1}{\mathrm{Vol}(V_b)}$ for the $a \neq b$ pair that shifts the argmin towards balanced pairs. For the above reasons, analogously to the ratio and normalized cuts, the following notions were introduced in [20].

Definition 7 *The balanced Newman-Girvan modularity corresponding to the k-partition $P_k = (V_1, \ldots, V_k)$ of the vertex-set of $G = (V, \boldsymbol{W})$ ($\mathrm{Vol}(V) = 1$) is*

$$BM(P_k, G) = \sum_{a=1}^{k} \frac{1}{|V_a|} \sum_{i,j \in V_a} (w_{ij} - d_i d_j) = \sum_{a=1}^{k} \left[\frac{e(V_a, V_a)}{|V_a|} - \frac{\mathrm{Vol}^2(V_a)}{|V_a|} \right]$$

and the balanced k-module Newman-Girvan modularity of G is

$$BM_k(G) = \max_{P_k \in \mathcal{P}_k} BM(P_k, G).$$

Definition 8 *The normalized Newman-Girvan modularity corresponding to the k-partition $P_k = (V_1, \ldots, V_k)$ of the vertex-set of $G = (V, \boldsymbol{W})$ ($\mathrm{Vol}(V) = 1$) is*

$$NM(P_k, G) = \sum_{a=1}^{k} \frac{1}{\mathrm{Vol}(V_a)} \sum_{i,j \in V_a} (w_{ij} - d_i d_j) = \sum_{a=1}^{k} \frac{e(V_a, V_a)}{\mathrm{Vol}(V_a)} - 1$$

and he normalized k-module Newman-Girvan modularity of G is

$$NM_k(G) = \max_{P_k \in \mathcal{P}_k} NM(P_k, G).$$

Here we used the fact that $\sum_{a=1}^{k} \mathrm{Vol}(V_a) = 1$. In view of (1), minimizing the normalized cut of G over k-partitions of its vertices is equivalent to maximizing $\sum_{a=1}^{k} \frac{e(V_a, V_a)}{\mathrm{Vol}(V_a)}$. Hence, maximizing the normalized Newman–Girvan modularity can be solved with the same spectral method (using the normalized Laplacian) as the normalized cut problem. However, we introduce another method based on the normalized modularity matrix.

We also want to show another insight into the problem of the choice of k from the point of view of computational demand and by using the linear algebraic structure of our objective function. In this way, we will prove that for the selected k, maximizing the above adjusted modularities is equivalent to minimizing the k-variance of the vertex representatives by choosing an appropriate representation; hence, the k-means algorithm is applicable.

3.1 Maximizing the balanced Newman–Girvan modularity

The k-partition P_k is uniquely defined by the $n \times k$ balanced partition matrix $\boldsymbol{Z}_k = (\mathbf{z}_1, \ldots, \mathbf{z}_k)$, i.e.

$$BM(P_k, G) = \sum_{a=1}^{k} \mathbf{z}_a^T \boldsymbol{M} \mathbf{z}_a = \mathrm{tr}(\boldsymbol{Z}_k^T \boldsymbol{M} \boldsymbol{Z}_k)$$

where $\boldsymbol{M}$ is the modularity matrix. We want to maximize $\mathrm{tr}(\boldsymbol{Z}_k^T \boldsymbol{M} \boldsymbol{Z}_k)$ over balanced k-partition matrices $\boldsymbol{Z}_k \in \mathcal{Z}_k^B$. Since $\boldsymbol{Z}_k$ is a suborthogonal matrix, $\boldsymbol{Z}_k^T \boldsymbol{Z}_k = \boldsymbol{I}_k$.

Let $\beta_1 \geq \cdots \geq \beta_n$ denote the eigenvalues of the modularity matrix $\boldsymbol{M}$ with corresponding unit-norm, pairwise orthogonal eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_n$. Let p denote the number of its positive eigenvalues; thus, $\beta_{p+1} = 0$ and $\mathbf{u}_{p+1} = \mathbf{1}/\sqrt{n}$. Now let $\boldsymbol{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_k)$ be an arbitrary $n \times k$ suborthogonal matrix ($k \leq p$). Then

$$\max_{\boldsymbol{Z}_k \in \mathcal{Z}_k^B} BM(\boldsymbol{Z}_k, G) \leq \max_{\boldsymbol{Y}^T\boldsymbol{Y} = \boldsymbol{I}_k} \operatorname{tr}(\boldsymbol{Y}^T\boldsymbol{M}\boldsymbol{Y}) = \sum_{a=1}^{k} \beta_a \leq \sum_{a=1}^{p+1} \beta_a. \tag{28}$$

Both inequalities can be attained by equality only in the $k = 1$, $p = 0$ case, when our underlying graph is the complete graph. In this case there is only one cluster with partition vector of equal coordinates (balanced eigenvector corresponding to the single 0 eigenvalue). For $k > 1$, partition vectors for no graph can coincide with eigenvectors corresponding to positive eigenvalues, since their coordinates do not sum to zero that would be necessary to be orthogonal to the vector corresponding to the 0 eigenvalue.

It is also obvious that the maximum with respect to k of the maximum in (28) is attained with the choice of $k = p + 1$. In [62], for the non-penalized case, the author shows how $p + 1$ clusters can be constructed by applying a vector partitioning algorithm for $\mathbf{u}_1, \ldots, \mathbf{u}_p$. However, in case of large networks, p can also be large, and computation of the positive eigenvalues together with eigenvectors is time-consuming. As a compromise, it will be shown that choosing a $k < p$ such that there is a remarkable gap between β_{k-1} and β_k will also suffice. Further, even for a fixed "small" $k < p$, to find the true maxim over k-partitions cannot be solved in polynomial time in n, but due to our estimations, spectral partitioning algorithms can be constructed like spectral clustering based on Laplacian eigenvectors. Now, we are going to discuss this issue in details.

We expand $BM(P_k, G)$ with respect to the eigenvalues and eigenvectors of the modularity matrix:

$$BM(P_k, G) = \operatorname{tr}(\boldsymbol{Z}_k^T\boldsymbol{M}\boldsymbol{Z}_k) = \sum_{a=1}^{k} \mathbf{z}_a^T(\sum_{i=1}^{n} \beta_i \mathbf{u}_i\mathbf{u}_i^T)\mathbf{z}_a = \sum_{i=1}^{n} \beta_i \sum_{a=1}^{k} (\mathbf{u}_i^T\mathbf{z}_a)^2.$$

We can increase the last sum if we neglect the terms corresponding to the negative eigenvalues, hence, the outer summation stops at p, or equivalently, at $p + 1$. In this case the inner sum is the largest if $k = p + 1$, when the partition vectors $\mathbf{z}_1, \ldots, \mathbf{z}_{p+1}$ are 'close' to the eigenvectors $\mathbf{u}_1, \ldots, \mathbf{u}_{p+1}$, respectively. As both systems consist of orthonormal sets of vectors, the two subspaces spanned by them should be close to each other. The subspace $F_{p+1} = \operatorname{Span}\{\mathbf{z}_1, \ldots, \mathbf{z}_{p+1}\}$ consists of piecewise constant vectors on $p+1$ steps, therefore $\mathbf{u}_{p+1} \in F_{p+1}$, and it suffices to process only the first p eigenvectors. The notation $Q_{p+1,p}$ will be used for the increased objective function based on the first p eigenvalue–eigenvector pairs and looking for $p + 1$ clusters:

$$BM(P_{p+1}, G) \leq Q_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M}) := \sum_{i=1}^{p} \beta_i \sum_{a=1}^{p+1} (\mathbf{u}_i^T\mathbf{z}_a)^2.$$

In the sequel, for given $\boldsymbol{M}$, we want to maximize $Q_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M})$ over $\mathcal{Z}_{p+1}^B$.

For this purpose, let us project the vectors $\sqrt{\beta_i}\mathbf{u}_i$ onto the subspace F_{p+1}:

$$\sqrt{\beta_i}\mathbf{u}_i = \sum_{a=1}^{p+1} [(\sqrt{\beta_i}\mathbf{u}_i)^T\mathbf{z}_a]\mathbf{z}_a + \operatorname{ort}_{\mathcal{F}_{p+1}}(\sqrt{\beta_i}\mathbf{u}_i), \quad i = 1, \ldots, p. \tag{29}$$

The first term is the component in the subspace, and the second is orthogonal to it. In fact, the projected copies will be in a p-dimensional subspace of F_{p+1} orthogonal to the $\mathbf{1}$ vector (scalar multiple of $\mathbf{u}_{p+1}$). They will be piecewise constant vectors on $p+1$ steps, and their coordinates sum to 0. This is why one less eigenvectors are used than the number of clusters looked for.

By the Pythagorean theorem, for the squared lengths of the vectors in the decomposition (29) we get that

$$\beta_i = \|\sqrt{\beta_i}\mathbf{u}_i\|^2 = \sum_{a=1}^{p+1}[(\sqrt{\beta_i}\mathbf{u}_i)^T\mathbf{z}_a]^2 + \mathrm{dist}^2(\sqrt{\beta_i}\mathbf{u}_i, F_{p+1}), \quad i = 1,\dots,p.$$

By summing for $i = 1,\dots,p$, the cumulated second term will turn out to be the sum of inner variances of the vertex representatives in the representation, defined as follows. For a given positive integer $d \le p$, let the d-dimensional representatives $\mathbf{x}_1,\dots,\mathbf{x}_n$ of the vertices be row vectors of the $n \times d$ matrix $\boldsymbol{X}_d = (\sqrt{\beta_1}\mathbf{u}_1,\dots,\sqrt{\beta_d}\mathbf{u}_d)$. Their k-variance is $S_k^2(\boldsymbol{X}_d)$. Since F_k consists of piecewise constant vectors on the partition $(V_1,\dots,V_k)$, by thee ANOVA argument it follows that

$$S_k^2(\boldsymbol{X}_d) = \sum_{i=1}^{d}\mathrm{dist}^2(\sqrt{\beta_i}\mathbf{u}_i, F_k).$$

Hence,

$$\begin{aligned}\sum_{i=1}^{p}\beta_i &= \sum_{i=1}^{p}\sum_{a=1}^{p+1}[(\sqrt{\beta_i}\mathbf{u}_i)^T\mathbf{z}_a]^2 + \sum_{i=1}^{p}\mathrm{dist}^2(\sqrt{\beta_i}\mathbf{u}_i, F_{p+1}) \\ &= Q_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M}) + S_{p+1}^2(\boldsymbol{X}_p),\end{aligned}$$

where the rows of $\boldsymbol{X}_p = (\sqrt{\beta_1}\mathbf{u}_1,\dots,\sqrt{\beta_p}\mathbf{u}_p)$ are p-dimensional representatives of the vertices. We could as well take $(p+1)$-dimensional representatives as the last coordinates are zeros, and hence, $S_{p+1}^2(\boldsymbol{X}_p) = S_{p+1}^2(\boldsymbol{X}_{p+1})$. Thus, maximizing $Q_{p+1,p}$ is equivalent to minimizing $S_{p+1}^2(\boldsymbol{X}_p)$ that can be obtained by applying the k-means algorithm for the p-dimensional representatives with $p+1$ clusters.

More generally, if there is a gap between β_d and $\beta_{d+1} > 0$, then we may look for k clusters based on d-dimensional representatives of the vertices. Analogously to the above calculations, for $d < k \le p+1$ we have that

$$\begin{aligned}\sum_{i=1}^{d}\beta_i &= \sum_{i=1}^{d}\sum_{a=1}^{k}[(\sqrt{\beta_i}\mathbf{u}_i)^T\mathbf{z}_a]^2 + \sum_{i=1}^{d}\mathrm{dist}^2(\sqrt{\beta_i}\mathbf{u}_i, F_k) \\ &=: Q_{k,d}(\boldsymbol{Z}_k, \boldsymbol{M}) + S_k^2(\boldsymbol{X}_d).\end{aligned} \tag{30}$$

If β_d is much greater than β_{d+1}, the k-variance $S_k^2(\boldsymbol{X}_{d+1})$ is not significantly greater than $S_k^2(\boldsymbol{X}_d)$, since $\boldsymbol{X}_{d+1}$'s last column, $\sqrt{\beta_{d+1}}\mathbf{u}_{d+1}$, will not increase too much the k-variance of the d-dimensional representatives, its norm being much less than that of the first d columns. As the left hand side of (30) is not increased significantly by adding β_{d+1}, the quantity $Q_{k,d+1}(\boldsymbol{Z}_k, \boldsymbol{M})$ is not much greater than $Q_{k,d}(\boldsymbol{Z}_k, \boldsymbol{M})$ is. Neither the classification nor the value of the modularity is changed much compared to the cost of taking one more eigenvector into consideration. After d has been selected, we can process the

k-means algorithm with $k = d+1, \ldots, p+1$ clusters. By an easy argument, $S^2_{k+1}(\boldsymbol{X}_d) \le S^2_k(\boldsymbol{X}_d)$, but we can stop, if it is much less. These considerations would minimize computational demand and proved good for randomly generated graphs from different block structures, see Chapter **??**.

Calculating eigenvectors is costly; the Lánczos method (see e.g. [35]) performs well if we calculate only eigenvectors corresponding to some leading eigenvalues followed by a spectral gap. In [7, 42], the authors suggest to use as many eigenvectors as possible. In fact, using more eigenvectors (up to p) is better from the point of view of accuracy, but using less eigenvectors (up to a gap in the positive part of the spectrum) is better from the computational point of view, cf. [64, 59]. We have to compromise. By these arguments, a local maximum of the modularity can be expected at $k = d+1$.

The advantage of the modularity matrix versus the Laplacian is that here 0 is a watershed, and for small graphs, the $d = p$, $k = p+1$ choice is feasible; for large graphs we look for gaps (like in case of the Laplacian) in the positive part of the modularity spectrum, and the number of clusters is one more than the number of the largest positive eigenvalues with corresponding eigenvectors entered into the classification.

3.2 Maximizing the normalized Newman–Girvan modularity

The k-partition P_k is also uniquely defined by the $n \times k$ normalized partition matrix $\boldsymbol{Z}_k = (\mathbf{z}_1, \ldots, \mathbf{z}_k)$ introduced in (4). With it,

$$NM(P_k, G) = \sum_{a=1}^{k} \mathbf{z}_a^T \boldsymbol{M} \mathbf{z}_a = \mathrm{tr}[(\boldsymbol{D}^{1/2}\boldsymbol{Z}_k)^T \boldsymbol{M}_D (\boldsymbol{D}^{1/2}\boldsymbol{Z}_k)]$$

where $\boldsymbol{M}_D$ is the normalized modularity matrix defined in Lesson 2. Since the matrix $\boldsymbol{D}^{1/2}\boldsymbol{Z}_k$ is suborthogonal, the maximization here happens with respect to $\boldsymbol{Z}_k^T \boldsymbol{D} \boldsymbol{Z}_k = \boldsymbol{I}_k$, that is over normalized k-partition matrices $\boldsymbol{Z}_k \in \mathcal{Z}_k^N$.

Let $\beta'_1 \ge \cdots \ge \beta'_n$ denote the eigenvalues of the symmetric normalized modularity matrix $\boldsymbol{M}_D$ with corresponding unit-norm, pairwise orthogonal eigenvectors $\mathbf{u}'_1, \ldots, \mathbf{u}'_n$. We saw that the spectrum of $\boldsymbol{M}_D$ is in $[-1, 1]$ and includes the 0.

Let p denote the number of positive eigenvalues of $\boldsymbol{M}_D$ (this p not necessarily coincides with that of Section 3.1). Now let $\boldsymbol{Y} = (\mathbf{y}_1, \ldots, \mathbf{y}_k)$ be an arbitrary $n \times k$ matrix ($k \le p$) such that $\boldsymbol{Y}^T \boldsymbol{D} \boldsymbol{Y} = \boldsymbol{I}_k$. With the same linear algebra as used in Section 3.1,

$$\max_{\boldsymbol{Z}_k \in \mathcal{Z}_k^n} NM(P_k, G) \le \max_{\boldsymbol{Y}^T \boldsymbol{D} \boldsymbol{Y} = \boldsymbol{I}_k} \mathrm{tr}(\boldsymbol{Y}^T \boldsymbol{M} \boldsymbol{Y}) \le \sum_{a=1}^{k} \beta'_a \le \sum_{a=1}^{p+1} \beta'_a.$$

For further investigation, we expand our objective function with respect to the eigenvectors:

$$NM(P_k, G) = \sum_{i=1}^{n} \beta'_i \sum_{a=1}^{k} [(\mathbf{u}'_i)^T (\boldsymbol{D}^{1/2}\mathbf{z}_a)]^2.$$

We can increase this sum if we neglect the terms corresponding to the negative eigenvalues, hence, the outer summation stops at p, or equivalently, at $p+$

1. The inner sum is the largest in the $k = p + 1$ case, when the unit-norm, pairwise orthogonal vectors $\boldsymbol{D}^{1/2}\mathbf{z}_1, \ldots, \boldsymbol{D}^{1/2}\mathbf{z}_{p+1}$ are close to the eigenvectors $\mathbf{u}'_1, \ldots, \mathbf{u}'_{p+1}$, respectively. In fact, the two subspaces spanned by them should be close to each other. Now the subspace $F_{p+1} = \mathrm{Span}\{\boldsymbol{D}^{1/2}\mathbf{z}_1, \ldots, \boldsymbol{D}^{1/2}\mathbf{z}_{p+1}\}$ does not consist of piecewise constant vectors, but the following argument is valid. By the notation $Q'_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M})$ for the increased objective function based on the first p eigenvalue–eigenvector pairs and looking for $p + 1$ clusters we get that

$$NM(P_{p+1}, G) \le Q'_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M}) := \sum_{i=1}^{p} \beta'_i \sum_{a=1}^{p+1} [(\mathbf{u}'_i)^T (\boldsymbol{D}^{1/2}\mathbf{z}_a)]^2.$$

In the sequel, for given $\boldsymbol{M}$, we want to maximize $Q'_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M})$ over $\mathcal{Z}^N_{p+1}$.

With the argument of Section 3.1, now the vectors $\sqrt{\beta'_i}\,\mathbf{u}'_i$ are projected onto the subspace F_{p+1}:

$$\sqrt{\beta'_i}\,\mathbf{u}'_i = \sum_{a=1}^{p+1} [(\sqrt{\beta'_i}\,\mathbf{u}'_i)^T \boldsymbol{D}^{1/2}\mathbf{z}_a]\, \boldsymbol{D}^{1/2}\mathbf{z}_a + \mathrm{ort}_{\mathcal{F}_{p+1}}(\sqrt{\beta'_i}\,\mathbf{u}'_i), \quad i = 1, \ldots, p.$$

As $\sqrt{\beta'_{p+1}}\,\mathbf{u}'_{p+1} = \mathbf{0}$, there is no use of projecting it.

By the Pythagorean theorem, for the squared lengths of the vectors in the above orthogonal decomposition we get that

$$\beta'_i = \|\sqrt{\beta'_i}\,\mathbf{u}'_i\|^2 = \sum_{a=1}^{p+1} [(\sqrt{\beta'_i}\,\mathbf{u}'_i)^T \boldsymbol{D}^{1/2}\mathbf{z}_a]^2 + \mathrm{dist}^2(\sqrt{\beta'_i}\,\mathbf{u}'_i, F_{p+1}), \quad i = 1, \ldots, p.$$

Let the vertex representatives $\mathbf{x}'_1, \ldots, \mathbf{x}'_n \in \mathbb{R}^p$ be the row vectors of the $n \times p$ matrix $\boldsymbol{X}'_p = (\sqrt{\beta'_1}\,\boldsymbol{D}^{-1/2}\mathbf{u}'_1, \ldots, \sqrt{\beta'_p}\,\boldsymbol{D}^{-1/2}\mathbf{u}'_p)$. Then

$$\mathrm{dist}^2(\sqrt{\beta'_i}\,\mathbf{u}'_i, F_{p+1}) = \sum_{j=1}^{n} d_j (x'_{ji} - c_{ji})^2, \quad i = 1, \ldots, p$$

where x'_{ji} is the ith coordinate of the vector $\mathbf{x}'_j$ and c_{ji} is the same for the vector $\mathbf{c}_j \in \mathbb{R}^p$, where there are at most $p + 1$ different ones among the centers $\mathbf{c}_1, \ldots, \mathbf{c}_n$ assigned to the vertex representatives. Namely,

$$c_{ji} = \frac{1}{\sum_{\ell \in V_a} d_\ell} \sum_{\ell \in V_a} d_\ell x'_{\ell i}, \quad j \in V_a, \quad i = 1, \ldots, p.$$

In other words, the column vectors of the $n \times p$ matrix of rows $\mathbf{c}_1, \ldots, \mathbf{c}_n$ are stepwise constant vectors on the same $p + 1$ steps corresponding to the $(p + 1)$-partition of the vertices encoded into the partition matrix $\boldsymbol{Z}_{p+1}$.

By summing for $i = 1, \ldots, p$, in view of the ANOVA argument of Section 3.1, the cumulated second term will turn out to be the weighted $(p + 1)$-variance of the vertex representatives in the $(p + 1)$-partition designated by the partition matrix $\boldsymbol{Z}_{p+1}$:

$$\tilde{S}^2_{p+1}(\boldsymbol{X}'_p) = \sum_{i=1}^{p} \mathrm{dist}^2(\sqrt{\beta'_i}\,\mathbf{u}'_i, F_{p+1}) = \sum_{j=1}^{n} d_j \|\mathbf{x}_j - \mathbf{c}_j\|^2.$$

Therefore,

$$\sum_{i=1}^{p} \beta'_i = Q'_{p+1,p}(\boldsymbol{Z}_{p+1}, \boldsymbol{M}) + \tilde{S}^2_{p+1}(\boldsymbol{X}'_p).$$

This applies to a given $(p+1)$-partition of the vertices. We are looking for the $(p+1)$-partition maximizing the first term. In view of the above formula, increasing $Q'_{p+1,p}$ can be achieved by decreasing $\tilde{S}^2_{p+1}(\boldsymbol{X}'_p)$; latter one is obtained by applying the k-means algorithm with $p+1$ clusters for the p-dimensional representatives $\mathbf{x}'_1, \ldots, \mathbf{x}'_n$ with respective weights $d_1, \ldots, d_n$.

Analogously, for $d < k \leq p+1$:

$$\begin{aligned}\sum_{i=1}^{d} \beta'_i &= \sum_{i=1}^{d}\sum_{a=1}^{k} [(\sqrt{\beta'_i}\,\mathbf{u}'_i)^T \boldsymbol{D}^{1/2}\mathbf{z}_a]^2 + \sum_{i=1}^{d} \mathrm{dist}^2(\sqrt{\beta'_i}\,\mathbf{u}'_i, F_k) \\ &= Q'_{k,d}(\boldsymbol{Z}_k, \boldsymbol{M}) + \tilde{S}^2_k(\boldsymbol{X}'_d)\end{aligned}$$

where the row vectors of the $n \times d$ matrix $\boldsymbol{X}'_d = (\sqrt{\beta'_1}\,\boldsymbol{D}^{-1/2}\mathbf{u}'_1, \ldots, \sqrt{\beta'_d}\,\boldsymbol{D}^{-1/2}\mathbf{u}'_d)$ are d-dimensional representatives of the vertices. Hence, in the presence of a spectral gap between β'_d and $\beta'_{d+1} > 0$ – in the miniature world of the [0,1] interval – neither $\sum_{i=1}^{d} \beta'_i$ nor $\tilde{S}^2_k(\boldsymbol{X}'_d)$ can be increased significantly by introducing one more eigenvalue-eigenvector pair (by using $(d+1)$-dimensional representatives instead of d-dimensional ones). Consequently, $Q'_{k,d}(\boldsymbol{Z}_k, \boldsymbol{M})$ would not change much, and by the argument of Section 3.1, $k = d+1$ clusters based on d-dimensional representatives will suffice.

In their paper [43] introduce a model that takes into consideration the heterogeneity in the degrees of vertices. While the usual blockmodel is biased towards placing vertices of similar degrees in the same cluster, the new model is capable to find clusters of vertices of heterogeneous degrees. Similar stochastic blockmodels will be discussed later.

3.3 Anti-community structure

Given the weighted graph $G = (V, \boldsymbol{W})$, instead of taking the maximum, we take the minimum of $Q_B(P_k, \boldsymbol{W}) = Q_B(\boldsymbol{Z}_k, \boldsymbol{M})$ over balanced k-partition matrices $\boldsymbol{Z}_k$. For fixed $k \leq m$, analogously to the inference of Section 3.1,

$$\begin{aligned}\min_{P_k \in \mathcal{P}_k} BM(P_k, G) &= \min_{\boldsymbol{Z}_k^T \boldsymbol{Z}_k = \boldsymbol{I}_k} \mathrm{tr}(\boldsymbol{Z}_k^T \boldsymbol{M} \boldsymbol{Z}_k) \geq \min_{\boldsymbol{Y}^T \boldsymbol{Y} = \boldsymbol{I}_k} \mathrm{tr}(\boldsymbol{Y}^T \boldsymbol{M} \boldsymbol{Y}) \\ &\geq \sum_{a=1}^{k} \beta_{n+1-a} \geq \sum_{a=1}^{m+1} \beta_{n+1-a}\end{aligned}$$

where m is the number of negative eigenvalues of $\boldsymbol{M}$ ($m+p < n$). For the classification, here we use the scaled (by the square root of the absolute value of the corresponding eigenvalue) eigenvectors corresponding to the negative eigenvalues for the representation to find $m+1$ clusters. For large n, it suffices to choose $d < m$ structural negative eigenvalues such that there is a remarkable spectral gap between β_{n+1-d} and β_{n-d}. Then with $\boldsymbol{X}_d = (\sqrt{|\beta_n|}\mathbf{u}_n, \ldots, \sqrt{|\beta_{n+1-d}|}\mathbf{u}_{n+1-d})$, we find the minimum of $S^2_{d+1}(\boldsymbol{X}_d)$ by the k-means algorithm with $d+1$ clusters.

The same can be done by minimizing the normalized modularity based on the largest absolute value negative eigenvalues and the corresponding eigenvectors of

the normalized modularity matrix. The following examples illustrate that large positive eigenvalues of the modularity matrix are indications of a community, while large absolute value negative ones, of an anti-community structure. In [68], these structures are called 'homophilic' or 'heterophilic'. For the heterophilic structure an example is the network of dating relationships in a high school, where two persons of opposite sex are more likely to date than persons of the same sex.

(i) Let G be the disjoint union of k complete graphs $C_{n_1}, \ldots, C_{n_k}$, respectively, with total number of vertices $n = \sum_{i=1}^{k} n_i$ and corresponding partition $V_1, \ldots, V_k$ of the vertices. This is sometimes called *pure community structure*, since there are no inter-community edges, but all possible intra-community edges are present. The modularity matrix of G has $k-1$ positive eigenvalues, $\beta_k = 0$ with corresponding eigenvector $\mathbf{1}/\sqrt{n}$, and there is only one negative eigenvalue with multiplicity $n-k$. (In the $n_1 = \cdots = n_k$ special case $\beta_1 = \cdots = \beta_{k-1}$ is a multiple positive eigenvalue.) Here k communities are detected by the k-means algorithm applied for the $(k-1)$-dimensional representatives based on the eigenvectors corresponding to the positive eigenvalues. As these eigenvectors themselves have piecewise constant structures over the clusters $V_1, \ldots, V_k$, the k-variance of the representatives is 0, and the maximum $BM(P_k, G)$ is a slightly smaller positive number than the maximum $Q_{k,k-1}(\boldsymbol{Z}_k, \boldsymbol{M})$, latter one being the sum of the positive eigenvalues. In the $k = 1$ case the modularity matrix is negative semidefinite, and both the maximum $BM(P_k, G)$ and $Q_{k,k-1}(\boldsymbol{Z}_k, \boldsymbol{M})$ are zeros. The normalized modularity matrix $\boldsymbol{M}_D$ of G has the eigenvalue 1 with multiplicity $k-1$, one 0 eigenvalue and all the other eigenvalues are in the $(-1, 0)$ interval taking on at most $k-1$ different values. (In the $n_1 = \cdots = n_k$ case there is only one negative eigenvalue with multiplicity $n-k$.)

(ii) Let G be the complete k-partite graph $K_{n_1,\ldots,n_k}$, with total number of vertices $n = \sum_{i=1}^{k} n_i$ and corresponding partition $V_1, \ldots, V_k$ of the vertices. This is sometimes called *pure anti-community structure* as the empty modules may model hub-authorities and correspond to perfectly disassortative mixing. The modularity matrix of G has $k-1$ negative eigenvalues, all the other eigenvalues are zeros. (In the $n_1 = \cdots = n_k$ special case there is one negative eigenvalue with multiplicity $k-1$.) Here k communities are detected by the k-means algorithm applied for the $(k-1)$-dimensional representatives based on the eigenvectors corresponding to the negative eigenvalues. As these eigenvectors themselves have piecewise constant structures over the clusters $V_1, \ldots, V_k$, the k-variance of the representatives is 0, the minimum $BM(P_k, \boldsymbol{G})$ is negative, but slightly larger than the minimum $Q_{k,k-1}(\boldsymbol{Z}_k, \boldsymbol{M})$, latter one being the sum of the negative eigenvalues. The normalized modularity matrix $\boldsymbol{M}_D$ of G has $k-1$ negative eigenvalues in the $[-1, 0)$ interval, all the other eigenvalues are zeros. (In the $n_1 = \cdots = n_k$ case the only negative eigenvalue has multiplicity $k-1$.)

Note that the complete graph ((i) with $k = 1$) and complete k-partite graphs ((ii) with $k \geq 2$) have the zero as the largest modularity eigenvalue. Dragan

Stevanovic conjectures that these are the only graphs with a positive semidefinite modularity matrix (of which zero is always an eigenvalue). An extensive numerical search also supports this fact, though, it is an open question yet.

We remark that strategic interaction games also provide examples for both community and anti-community structures. Here the agents are vertices of a graph and agents connected with an edge (of non-zero weight) influence each other's actions, see e.g. [11, 40] for economic networks and simple graphs. The theory can be extended to edge-weighted graphs, where the impact of an agent's action on another agent's action depends on the edge-weight between them. The actions themselves are real numbers that – taking into consideration the graph structure – maximize the joint quadratic payoff which is of the following two types. In games of so-called *strategic complements*, an increase of the actions of other players leads a given player's higher actions to have relatively higher payoffs compared to that player's lower actions. In games of so-called *strategic substitutes* the opposite is true: an increase in other players' actions leads to relatively lower payoffs under higher actions of a given player. If we classify the agents such that those exhibiting similar actions belong to the same cluster, then a community and an anti-community structure is likely to develop in the two above cases, respectively. We may extend the theory to multiple actions, where the action vectors play a similar role than the representatives of the vertices in the quadratic placement problems of Lesson 1. For genetic applications consult [76]. For more examples see [20].

4 Normalized bicuts of contingency tables

[This section can be skipped.]

We are given an $m \times n$ contingency table $\boldsymbol{C}$ on row set Row and column set Col. For a fixed integer k, $0 < k \leq r = \text{rank}(\boldsymbol{C})$, we want to simultaneously partition the rows and columns of $\boldsymbol{C}$ into disjoint, nonempty subsets

$$Row = R_1 \cup \cdots \cup R_k, \quad Col = C_1 \cup \cdots \cup C_k$$

such that the cuts $c(R_a, C_b) = \sum_{i \in R_a} \sum_{j \in C_b} c_{ij}, \quad a, b = 1, \ldots, k$ between the row-column cluster pairs be as homogeneous as possible.

Definition 9 *The normalized bicut of the contingency table $\boldsymbol{C}$ with respect to the k-partitions $P_{row} = (R_1, \ldots, R_k)$ and $P_{col} = (C_1, \ldots, C_k)$ of its rows and columns and the collection of signs σ is defined as follows:*

$$\nu_k(P_{row}, P_{col}, \sigma) = \sum_{a=1}^{k} \sum_{b=1}^{k} \left(\frac{1}{\text{Vol}(R_a)} + \frac{1}{\text{Vol}(C_b)} + \frac{2\sigma_{ab}\delta_{ab}}{\sqrt{\text{Vol}(R_a)\text{Vol}(C_b)}} \right) c(R_a, C_b), \tag{31}$$

where

$$\text{Vol}(R_a) = \sum_{i \in R_a} d_{row,i} = \sum_{i \in R_a} \sum_{j=1}^{n} c_{ij}, \quad \text{Vol}(C_b) = \sum_{j \in C_b} d_{col,j} = \sum_{j \in C_b} \sum_{i=1}^{m} c_{ij}$$

are volumes of the clusters, δ_{ab} is the Kronecker delta, and the sign σ_{ab} is equal to 1 or -1 (it only has relevance in the $a = b$ case), and $\sigma = (\sigma_{11}, \ldots, \sigma_{kk})$ is the collection of the relevant signs.

The normalized k-way bicut of the contingency table $\boldsymbol{C}$ is the minimum of (31) over all possible k-partitions $\mathcal{P}_{row,k}$ and $\mathcal{P}_{col,k}$ of its rows and columns, and over all possible collections of signs σ:

$$\nu_k(\boldsymbol{C}) = \min_{P_{row},P_{col},\sigma} \nu_k(P_{row}, P_{col}, \sigma).$$

Note that $\nu_k(\boldsymbol{C})$ penalizes row- and column clusters of extremely different volumes in the $a \neq b$ case, whereas in the $a = b$ case σ_{aa} moderates the balance between $\mathrm{Vol}(R_a)$ and $\mathrm{Vol}(C_a)$.

Theorem 5 *Let $1 = s_0 \geq s_1 \geq \cdots \geq s_{r-1} > 0$ be the positive singular values of the normalized contingency table $\boldsymbol{C}_{corr} = \boldsymbol{D}_{row}^{-1/2}\boldsymbol{C}\boldsymbol{D}_{col}^{-1/2}$ belonging to $\boldsymbol{C}$. Then for any positive integer $k \leq r$, such that $s_{k-1} > s_k$,*

$$\nu_k(\boldsymbol{C}) \geq 2k - \sum_{i=0}^{k-1} s_i.$$

Proof 5 *We will show that $\nu_k(P_{row}, P_{col}, \sigma)$ is the objective function Q_k of (??) in the special representation, where the column vectors of $\boldsymbol{X}$ and $\boldsymbol{Y}$ are normalized partition vectors corresponding to P_{row} and P_{col}, respectively. From here, the statement follows, since the overall minimum is $2k - \sum_{i=0}^{k-1} s_i$. Indeed, denoting by x_{ia} the ith coordinate of the ath column of $\boldsymbol{X}$, in view of (4),*

$$x_{ia} = \begin{cases} \frac{1}{\sqrt{\mathrm{Vol}(R_a)}} & \text{if} \quad i \in R_a \\ 0 & \text{otherwise} \end{cases} \qquad (a = 1, \ldots, k).$$

Likewise, denoting by y_{jb} the jth coordinate of the bth column of $\boldsymbol{Y}$,

$$y_{jb} = \begin{cases} \frac{1}{\sqrt{\mathrm{Vol}(C_b)}} & \text{if} \quad j \in C_b \\ 0 & \text{otherwise} \end{cases}, \quad (b = 1, \ldots, k).$$

With this, the matrices $\boldsymbol{X}$ and $\boldsymbol{Y}$ satisfy the conditions imposed on the representatives. Actually, the row and column represenatives, $\mathbf{r}_1, \ldots \mathbf{r}_m \in \mathbb{R}^k$ and $\mathbf{q}_1, \ldots, \mathbf{q}_n \in \mathbb{R}^k$, are the row vectors of $\boldsymbol{X}$ and $\boldsymbol{Y}$, and it is easy to verify that

$$\|\mathbf{r}_i - \mathbf{q}_j\|^2 = \frac{1}{\mathrm{Vol}(R_a)} + \frac{1}{\mathrm{Vol}(C_b)} + \frac{2\sigma_{bb}\delta_{ab}}{\sqrt{\mathrm{Vol}(R_a)\mathrm{Vol}(C_b)}}, \quad \text{if} \quad i \in R_a,\, j \in C_b.$$

Note that we introduced $\boldsymbol{C}_{corr}$ as correspondence matrix belonging to $\boldsymbol{C}$. This matrix is used intensively in Correspondence Analysis. For further reading about Correspondence Analysis we recommend [30, 31] and [18]. If $\boldsymbol{C}$, or equaivalently, $\boldsymbol{C}_{corr}$ is non-decomposable, then 1 is a single singular value.

Observe, that in case of a symmetric contingency table, we get the same result with the representation, based on the eigenvectors corresponding to the largest absolute value eigenvalues of the normalized modularity matrix. However, $\nu_k(P_{row}, P_{col}, \sigma)$ cannot always be directly related to the normalized cut, except the following two special cases.

- When the $k-1$ largest absolute value eigenvalues of the normalized modularity matrix are all positive, or equivalently, if the k smallest eigenvalues

(including the zero) of the normalized Laplacian matrix are farther from 1 than any other eigenvalue which is greater than 1. In this case, the $k-1$ largest singular values (apart from the 1) of the correspondence matrix are identical to the $k-1$ largest eigenvalues of the normalized modularity matrix, and the left and right singular vectors are identical to the corresponding eigenvector with the same orientation. Consequently, for the k-dimensional (in fact, $(k-1)$-dimensional) row- and column-representatives $\mathbf{r}_i = \mathbf{q}_i$ $(i = 1, \ldots, n = m)$ holds. With the choice $\sigma_{bb} = 1$ $(b = 1, \ldots, k)$, the corresponding $\nu_k(\boldsymbol{C})$ is twice the normalized cut of our weighted graph in which weights of edges within the clusters do not count. In this special situation, the normalized bicut also favors k-partitions with low inter-cluster edge-densities (therefore, intra-cluster densities tend to be large, as they do not count in the objective function).

- When the $k-1$ largest absolute value eigenvalues of the normalized modularity matrix are all negative, then $\mathbf{r}_i = -\mathbf{q}_i$ for all $(k-1)$-dimensional row and column representatives, and any (but only one) of them can be the corresponding vertex representative. Now $\nu_k(\boldsymbol{C})$, which is attained with the choice $\sigma_{bb} = -1$ $(b = 1, \ldots, k)$, differs from the normalized cut in that it also counts the edge-weights within the clusters. Indeed, in the $a = b$, $R_a = C_a = V_a$ case

$$\|\mathbf{r}_i - \mathbf{q}_j\|^2 = \frac{1}{\mathrm{Vol}(V_a)} + \frac{1}{\mathrm{Vol}(V_b)} + \frac{2}{\sqrt{\mathrm{Vol}(V_a)\mathrm{Vol}(V_b)}} = \frac{4}{\mathrm{Vol}(V_a)}$$

  if $i, j \in V_a$. Here, by minimizing the normalized k-way cut, rather a so-called anti-community structure is detected in that $c(R_a, C_a) = c(V_a, V_a)$ is suppressed to compensate for the term $\frac{4}{\mathrm{Vol}(V_a)}$.

We remark that [27] treats this problem for two row- and column-clusters and minimizes another objective function such that it favors 2-partitions where $c(R_1, C_2)$ and $c(R_2, C_1)$ are small compared to $c(R_1, C_1)$ and $c(R_2, C_2)$. The solution is also given by the transformed left- and right-hand side singular vector pair corresponding to s_1. However, it is the objective function ν_k which best complies with the SVD of the correspondence matrix, and hence, gives the continuous relaxation of the normalized bicut minimization problem. The idea of Ding et al. could be naturally extended to the case of several, but the same number of row and column clusters, and it may work well in the keyword-document classification problem. Though, in some real-life problems, e.g., clustering genes and conditions of microarrays, we rather want to find clusters of similarly functioning genes that equally (not especially weakly or strongly) influence conditions of the same cluster; this issue discussed in details later. For further reading about microarrays, we recommend [37, 44, 65]. [25] also suggests a multipartition algorithm that runs the k-means algorithm simultaneously for the row- and column representatives.

References

[1] Ajtai M, Komlos J and Szemerédi E 1983 Sorting in $c \log n$ parallel steps. *Combinatorica* **3**, 1–9.

[2] Aldous DJ 1989 Lower bounds for covering times for reversible Markov chains and random walks on graphs. *J. Theor. Probab.* **2**, 91–100.

[3] Alon N 1986 Eigenvalues and expanders. *Combinatorica* **6** (2), 83–96.

[4] Alon N Milman VD 1985 λ_1, isoperimetric inequalities for graphs and superconcentrators. *J. Comb. Theory Ser. B* **38**, 73–88.

[5] Alon N Milman VD 1987 Better expanders and superconcentrators. *J. Algorithms* **8**, 337–347.

[6] Alon N and Sudakov B 2000 Bipartite subgraphs and the smallest eigenvalue. *Comb. Probab. Comput.* **9**, 1-12.

[7] Alpert CJ and Yao S.-Z 1995 Spectral partitioning: the more eigenvectors, the better. In *Proc. 32nd ACM/IEEE International Conference on Design Automation* (Preas BT, Karger PG, Nobandegani BS and Pedram M eds), pp. 195–200. Association of Computer Machinery, New York.

[8] Arora S, Barak B and Steurer D 2010 Subexponential algorithms for unique games and related problems. In *Proc. 51st IEEE Symposium on Foundations of Computer Science (FOCS 2010)*, pp. 563–572. Washington DC, USA, IEEE Computer Society.

[9] Azran A and Ghahramani Z 2006 Spectral methods for automatic multiscale data clustering. In *Proc. IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR 2006), New York NY* (Fitzgibbon A, Taylor CJ and Lecun Y eds), pp. 190–197. IEEE Computer Society, Los Alamitos, California.

[10] Babai L and Szegedy M 1992 Local expansion of symmetric graphs. *Comb. Probab. Comput.* **1**, 1–11.

[11] Ballester C, Calvó-Armengol A and Zenou Y 2006 Who's who in networks. Wanted: The key player. *Econometrica* **74** (5), 1403–1417.

[12] Bolla M 1989 Spectra, Euclidean representation, and vertex-colourings of hypergraphs. Preprint 78/1989, Mathematical Institute of the Hungarian Academy of Sciences.

[13] Bolla M and Tusnády G 1990 Spectra and colourings of weighted graphs. Preprint 52/1990, Mathematical Institute of the Hungarian Academy of Sciences.

[14] Bolla M 1993 Spectra and Euclidean representation of hypergraphs. *Discret. Math.* **117**, 19–39.

[15] Bolla M and Tusnády G 1994 Spectra and Optimal Partitions of Weighted Graphs. *Discret. Math.* **128**, 1–20.

[16] Bolla M and M.-Sáska G 2002 Isoperimetric properties of weighted graphs related to the Laplacian spectrum and canonical correlations. *Stud. Sci. Math. Hung.* **39**, 425–441.

[17] Bolla M and M.-Sáska G 2004 Optimization problems for weighted graphs and related correlation estimates. *Discret. Math.* **282**, 23–33.

[18] Bolla M, Friedl K and Krámli A 2010 Singular value decomposition of large random matrices (for two-way classification of microarrays). *J. Multivariate Anal.* **101**, 434–446.

[19] Bolla M 2011 Beyond the expanders. *Int. J. Comb.*, 787596.

[20] Bolla M 2011 Penalized versions of the Newman–Girvan modularity and their relation to multi-way cuts and k-means clustering. *Phys. Rev. E* **84**, 016108.

[21] Buser P 1984 On the bipartition of graphs. *Discret. Appl. Math.* **9**, 105–109.

[22] Cheeger J 1970 A lower bound for the smallest eigenvalue of the Laplacian. In *Problems in Analysis* (ed. R. C. Gunning), pp. 195–199. Princeton Univ. Press, Princeton NJ.

[23] Chung F 1997 *Spectral Graph Theory*, CBMS Regional Conference Series in Mathematics **92**. American Mathematical Society, Providence RI.

[24] Clauset A, Newman MEJ and Moore C 2004 Finding community structure in very large networks. *Phys. Rev. E* **70**, 066111.

[25] Dhillon IS 2001 Co-clustering documents and words using bipartite spectral graph partitioning. In *Proc. ACM Int. Conf. Knowledge Disc. Data Mining (KDD 2001)* (Provost FJ and Srikant R eds), pp. 269-274. Association for Computer Machinery, New York.

[26] Diaconis P and Stroock D 1991 Geometric bounds for eigenvalues of Markov chains. *Ann. Appl. Probab.* **1**, 36–62.

[27] Ding C, He X, Zha H, Gu M and Simon HD 2003 A minmax cut spectral method for data clustering and graph partitioning. Technical Report 54111, Lawrence Berkeley National Laboratory.

[28] Donath WE and Hoffman AJ 1973 Lower bounds for the partitioning of graphs. *IBM J. Res. Develop.* **17**, 420–425.

[29] Duch J and Arenas A 2005 Community detection in complex networks using extremal optimization. *Phys. Rev. E* **72**, 027104.

[30] Faust K 2005 Using correspondence analysis for joint displays of affiliation networks. In *Models and Methods in Social Network Analysis* Vol. 7, (Carrington PJ and Scott J eds), pp. 117–147. Cambridge Univ. Press, Cambridge.

[31] Faust K, Willert KE, Rowlee DD and Skvoretz J 2002 Scaling and statistical models for affiliation networks: Patterns of participation among Soviet politicians during the Brezhnev era. *Social Networks* **24**, 231–259.

[32] Fiedler M 1972 Bounds for eigenvalues of doubly stochastic matrices. *Linear Algebra Appl.* **5** (98), 299–310.

[33] Fiedler M 1973 Algebraic connectivity of graphs. *Czech. Math. J.* **23** (98), 298–305.

[34] Fortunato S 2010 Community detection in graphs. *Phys. Rep.* **486**, 75–174.

[35] Golub GH and Van Loan CF 1996 *Matrix Computations*, 3rd edn. Johns Hopkins University Press, Baltimore, MD.

[36] Hagen L and Kahng AB 1992 New spectral methods for ratio cut partitioning and clustering. *IEEE Trans. Comput. Aided Des.* **11**, 1074–1085.

[37] Higham DJ, Kalna G and Vass JK 2005 Analysis of the singular value decomposition as a tool for processing microarray expression data. In *Proceedings of ALGORITMY 2005* (Handlovicova A, Kriva Z and Sevcovic D eds), pp. 250–259. Bratislava.

[38] Hoffman AJ 1972 Eigenvalues and partitionings of the edges of a graph. *Linear Algebra Appl.* **5**, 137–146.

[39] Hoory S, Linial N and Widgerson A 2006 Expander graphs and their applications. *Bull. Amer. Math. Soc. (N. S.)* **43** (4), 439–561.

[40] Jackson MO and Zenou Y 2014 Games on Networks. To appear in the *Handbook of Game Theory* **4** (Young P and Zamir S eds). Elsevier Science.

[41] Juhász F and Mályusz K 1980 Problems of cluster analysis from the viewpoint of numerical analysis. In *Numerical Methods, Coll. Math. Soc. J. Bolyai* (ed. Rózsa P), Vol 22, pp. 405–415. North-Holland, Amsterdam.

[42] Kannan R, Vempala S and Vetta A 2004 On clusterings: Good, bad and spectral. *J. ACM* **51**, 497–515.

[43] Karrer B and Newman MEJ 2011 Stochastic blockmodels and community structure in networks. *Phys. Rev. E* **83**, 016107.

[44] Kluger Y, Basri R, Chang JT and Gerstein M 2003 Spectral biclustering of microarray data: coclustering genes and conditions. *Genome Res.* **13**, 703–716.

[45] Lee JR, Gharan SO and Trevisan L 2012 Multi-way spectral partitioning and higher-order Cheeger inequalities. In *Proc. 44th Annual ACM Symposium on the Theory of Computing (STOC 2012)*, pp. 1117–1130. New York NY.

[46] Louis A, Raghavendra P, Tetali P and Vempala S 2011 Algorithmic extension of Cheeger's inequality to higher eigenvalues and partitions. In *Approximation, Randomization and Combinatorial Optimization. Algorithms and Techniques. Lecture Notes in Computer Science* (Goldborg LA, Jansen K, Ravi R and Rolim JDP eds), Vol. 6845, pp 315-326. Springer.

[47] Louis A, Raghavendra P, Tetali P and Vempala S 2012 Many sparse cuts via higher eigenvalues. In *Proc. 44th Annual ACM Symposium on the Theory of Computing (STOC 2012)*, pp. 1131–1140. New York NY.

[48] Lovász L 1993 *Combinatorial Problems and Exercises.* Akadémiai Kiadó–North Holland, Budapest–Amsterdam.

[49] Lovász L 1993 Random walks on graphs: a survey. In *Combinatorics, Paul Erdős is Eighty. János Bolyai Society, Mathematical Studies* Vol. 2, pp. 1–46. Keszthely, Hungary.

[50] Lovász L and Winkler P 1995 Exact mixing in an unknown Markov chain. *Electron. J. Comb.* **2**, paper R15, 1–14.

[51] Lovász L and Simonovits M 1993 Random walks in a convex body and an improved volume algorithm. *Random Struct. Algorithms* **4**, 359–412.

[52] Lubotzky A 1994 Discrete graphs, expanging graphs, and invariant measures. (With an appendix by J. D. Rogawski). In *Progress in Mathematics* **125**, Birkhäuser Verlag, Basel.

[53] Lusseau D Schneider K Boisseau OJ Haase P Slooten E and Dawson SM 2003 The bottlenose dolphin community of Doubtful Sound features a large proportion of long-lasting associations. *Behav. Ecol. Sociobiol.* **54**, 396–405.

[54] Meila M and Shi J 2001 Learning segmentation by random walks. In *Proc. 13th Neural Information Processing Systems Conference (NIPS 2001)* (Leen TK, Dietterich TG and Tresp V eds), pp. 873–879. MIT Press, Cambridge, USA.

[55] Mohar B 1988 Isoperimetric inequalities, growth and the spectrum of graphs. *Linear Algebra Appl.* **103**, 119–131.

[56] Mohar B 1989 Isoperimetric numbers of graphs. *J. Comb. Theor, Ser. B* **47**, 274–291.

[57] Mohar B and Poljak S 1990 Eigenvalues and the max-cut problem. *Czech. Math. J.* **40**, 343–352.

[58] Newman MEJ and Girvan M 2004 Finding and evaluating community structure in networks. *Phys. Rev. E* **69**, 026113.

[59] Newman MEJ 2004 Detecting community structure in networks. *Eur. Phys. J. B* **38**, 321–333.

[60] Newman MEJ 2004 Fast algorithm for detecting community structure in networks. *Phys. Rev. E* **69**, 066133.

[61] Newman MEJ 2004 Analysis of weighted networks. *Phys. Rev. E* **70**, 056131.

[62] Newman MEJ 2006 Finding community structure in networks using the eigenvectors of matrices. *Phys. Rev. E* **74**, 036104.

[63] Newman MEJ 2010 *Networks, An Introduction.* Oxford University Press.

[64] Ng AY Jordan MI and Weiss Y 2001 On spectral clustering: analysis and an algorithm. In *Proc. 14th Neural Information Processing Systems Conference (NIPS 2001)* (Dietterich TG, Becker S and Ghahramani Z eds), pp. 849–856. MIT Press, Cambridge, USA.

[65] Omberg L, Golub GH and Alter O 2007 A tensor higher-order singular value decomposition for integrative analysis of DNA microarray data from different studies. *Proc. Natl. Acad. Sci. USA* **104** (47), 18371–18376.

[66] Pólya G and Szegő S 1951 Isoperimetric inequalities in mathematical physics, *Ann. Math. Studies* **27**, Princeton University Press.

[67] Reichardt J. and Bornholdt S 2007 Partitioning and modularity of graphs with arbitrary degree distribution. *Phys. Rev. E* **76**, 015102(R).

[68] Rohe K, Chatterjee S and Yu B 2011 Spectral clustering and the high-dimensional stochastic blockmodel. *Ann. Stat.* **39** (4), 1878–1915.

[69] Sinclair A and Jerrum M 1989 Approximate counting, uniform generation and rapidly mixing Markov chains. *Inf. Comput.* **82**, 93–133.

[70] Telcs A 2006 *The Art of Random Walks*. Lecture Notes in Mathematics 1885, Springer.

[71] Tetali P 1991 Random walks and effective resistance of networks. *J. Theor. Probab.* **1**, 101–109.

[72] Thomassen C 1990 Resistances and currents in infinite electrical networks. *J. Comb. Theory* **49**, 87–102.

[73] Trevisan L 2009 Max cut and the smallest eigenvalue. In *Proc. 41th Annual ACM Symposium on the Theory of Computing (STOC 2009)*, pp. 1117–1130. Bethesda, Maryland USA.

[74] Von Luxburg U 2006 A tutorial on spectral clustering. *Stat. Comput.* **17**, 395–416.

[75] White S and Smyth P 2005 A spectral clustering approach to find communities in graphs. In *Proc. 5th SIAM International Conference on Data Mining* (Kargupta H, Srivastava J, Kamath C and Goodman A eds), pp. 274–285. Newport Beach, California.

[76] Wilkinson DM and Huberman BA 2004 A method for finding communities of related genes. *Proc. Natl. Acad. Sci. USA* **101** (50), 5241–5248.

[77] Zachary WW 1977 An information flow model for conflict and fission in small groups. *J. Antropol. Res.* **33**, 452–473.