

Newman 2006, Phys. Rev. E 74, 036104 – Published 11 September 2006
 “Finding community structure in networks using the eigenvectors of matrices”
<https://arxiv.org/pdf/physics/0605087.pdf>

n vertices, m edges
 assume that the network is a simple graph, having at most one edge between any pair of vertices and no self-edges

First, the algorithm which divides each subgraph into 2, iteratively.

M. E. J. Newman, Modularity and community structure in networks. Preprint physics/0602124 (2006).

Caveat: certain failure to find optimal modularity in some cases.

We begin by defining the adjacency matrix **A** to be the matrix with elements

$$A_{ij} = \begin{cases} 1 & \text{if there is an edge joining vertices } i, j, \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

(We restrict our attention in this paper to undirected networks, so that **A** is symmetric.) Then the number of edges *R* running between our two groups of vertices, also called the *cut size*, is given by

$$R = \frac{1}{2} \sum_{\substack{i, j \text{ in} \\ \text{different} \\ \text{groups}}} A_{ij}, \tag{2}$$

where the factor of $\frac{1}{2}$ compensates for our counting each edge twice in the sum.

To put this in a more convenient form, we define an *index vector* **s** with *n* elements

$$s_i = \begin{cases} +1 & \text{if vertex } i \text{ belongs to group 1,} \\ -1 & \text{if vertex } i \text{ belongs to group 2.} \end{cases} \tag{3}$$

(Note that **s** satisfies the normalization condition $\mathbf{s}^T \mathbf{s} = n$.)

$$\frac{1}{2}(1 - s_i s_j) = \begin{cases} 1 & \text{if } i \text{ and } j \text{ are in different groups,} \\ 0 & \text{if } i \text{ and } j \text{ are in the same group,} \end{cases} \tag{4}$$

which allows us to rewrite Eq. (2) as

$$R = \frac{1}{4} \sum_{ij} (1 - s_i s_j) A_{ij}. \tag{5}$$

Noting that the number of edges *k_i* connected to a vertex *i*—also called the *degree* of the vertex—is given by

$$k_i = \sum_j A_{ij}, \tag{6}$$

the first term of the sum in (5) is

$$\sum_{ij} A_{ij} = \sum_i k_i = \sum_i s_i^2 k_i = \sum_{ij} s_i s_j k_i \delta_{ij}, \tag{7}$$

where we have made use of $s_i^2 = 1$ (since $s_i = \pm 1$), and δ_{ij} is 1 if $i = j$ and zero otherwise. Thus

$$R = \frac{1}{4} \sum_{ij} s_i s_j (k_i \delta_{ij} - A_{ij}). \tag{8}$$

We can write this in matrix form as

$$R = \frac{1}{4} \mathbf{s}^T \mathbf{L} \mathbf{s}, \tag{9}$$

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where \mathbf{L} is the real symmetric matrix with elements $L_{ij} = k_i \delta_{ij} - A_{ij}$, or equivalently¹

$$L_{ij} = \begin{cases} k_i & \text{if } i = j, \\ -1 & \text{if } i \neq j \text{ and there is an edge } (i, j), \\ 0 & \text{otherwise.} \end{cases} \quad (10)$$

\mathbf{L} is called the *Laplacian matrix* of the graph or sometimes the *admittance matrix*. It appears in many contexts

Our task is to choose the vector \mathbf{s} so as to minimize the cut size, Eq. (9).

\mathbf{v}_i = normalized eigenvectors of \mathbf{L}

write \mathbf{s} as a linear combination of \mathbf{v}_i :

$\mathbf{s} = \sum_{i=1}^n a_i \mathbf{v}_i$, where $a_i = \mathbf{v}_i^T \mathbf{s}$ and the normalization $\mathbf{s}^T \mathbf{s} = n$ implies that

$$\sum_{i=1}^n a_i^2 = n. \quad (11)$$

$$R = \sum_i a_i \mathbf{v}_i^T \mathbf{L} \sum_j a_j \mathbf{v}_j = \sum_{ij} a_i a_j \lambda_j \delta_{ij} = \sum_i a_i^2 \lambda_i, \quad (12)$$

where λ_i is the eigenvalue of \mathbf{L} corresponding to the eigenvector \mathbf{v}_i and we have made use of $\mathbf{v}_i^T \mathbf{v}_j = \delta_{ij}$.

The sum of every row (and column) of the Laplacian matrix is zero:

$$\sum_j L_{ij} = \sum_j (k_i \delta_{ij} - A_{ij}) = k_i - k_i = 0, \quad (13)$$

where we have made use of (6). Thus the vector $(1, 1, 1, \dots)$ is always an eigenvector of the Laplacian with eigenvalue zero. It is less trivial, but still straightforward, to demonstrate that all eigenvalues of the Laplacian are nonnegative. (The Laplacian is symmetric and equal to the square of the edge incidence matrix, and hence its eigenvalues are all the squares of real vectors.) Thus the eigenvalue 0 is always the smallest eigenvalue of the Laplacian and the corresponding eigenvector is $\mathbf{v}_1 = (1, 1, 1, \dots)/\sqrt{n}$, correctly normalized.

Given these observations it is now straightforward to see how to minimize the cut size R . If we choose $\mathbf{s} = (1, 1, 1, \dots)$, then all of the weight in the final sum in Eq. (12) is in the term corresponding to the lowest eigenvalue $\lambda_1 = 0$ and all other terms are zero, since $(1, 1, 1, \dots)$ is an eigenvector and the eigenvectors are orthogonal. Thus this choice gives us $R = 0$, which is the smallest value it can take since it is by definition a non-negative quantity.

==> spectral partitioning is a poor approach for detecting natural community structure in real-world networks,

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modularity Q $Q = (\text{number of edges within communities})$
 $- (\text{expected number of such edges}). \quad (17)$

null model must have the same number of vertices n as the original network.
 We here consider the broad class of randomized models in which we specify separately the probability P_{ij} for an edge to fall between every pair of vertices i, j. More precisely, P_{ij} is the expected number of edges between i and j, a definition that allows for the possibility that there may be more than one edge between a pair of vertices, which happens in certain types of networks. We will consider some particular choices of P_{ij} in a moment, but for now let us pursue the developments in general form.

community. Let us define g_i to be the community to which vertex i belongs. Then the modularity can be written

$$Q = \frac{1}{2m} \sum_{ij} [A_{ij} - P_{ij}] \delta(g_i, g_j), \quad (18)$$

where δ(r, s) = 1 if r = s and 0 otherwise and m is again the number of edges in the network. The extra factor of

Returning to the null model, how should P_{ij} be chosen?
 undirected networks implies that P_{ij} = P_{ji}
 Q = 0 when all vertices are placed in a single group together:
 by definition, the nEdges within groups and expected nEdges == m
 Setting all g_i equal in Eq. (18), we find that P_{ij} [A_{ij} – P_{ij}] = 0 or equivalently

$$\sum_{ij} P_{ij} = \sum_{ij} A_{ij} = 2m. \quad (19)$$

$$P_{ij} = \frac{k_i k_j}{2m}. \quad (23)$$

This model has been studied in the past in its own right as a model of a network, for instance by Chung and Lu [62]. It is also closely related to the *configuration model*, which has been studied widely in the mathematics and physics literature [62, 63, 64, 65]. Indeed, essentially all expected properties of our model and the configuration model are identical in the limit of large network size, and hence Eq. (23) can be considered equivalent to the configuration model in this limit.²



A. Leading eigenvector method

As before, let us consider initially the division of a network into just two communities and denote a potential such division by an index vector \mathbf{s} with elements as in Eq. (3). We notice that the quantity $\frac{1}{2}(s_i s_j + 1)$ is 1 if i and j belong to the same group and 0 if they belong to different groups or, in the notation of Eq. (18),

$$\delta(g_i, g_j) = \frac{1}{2}(s_i s_j + 1). \tag{24}$$

Thus we can write (18) in the form

$$\begin{aligned} Q &= \frac{1}{4m} \sum_{ij} [A_{ij} - P_{ij}] (s_i s_j + 1) \\ &= \frac{1}{4m} \sum_{ij} [A_{ij} - P_{ij}] s_i s_j, \end{aligned} \tag{25}$$

This result can conveniently be rewritten in matrix form as

$$Q = \frac{1}{4m} \mathbf{s}^T \mathbf{B} \mathbf{s}, \tag{26}$$

where \mathbf{B} is the real symmetric matrix having elements

$$B_{ij} = A_{ij} - P_{ij}. \tag{27}$$

We call this matrix the *modularity matrix* and it plays

modularity matrix. Equations (6) and (20) together imply that all rows (and columns) of the modularity matrix sum to zero:

$$\sum_j B_{ij} = \sum_j A_{ij} - \sum_j P_{ij} = k_i - k_i = 0. \tag{28}$$

Unlike the Laplacian however, the eigenvalues of the modularity matrix are not necessarily all of one sign and in practice the matrix usually has both positive and negative eigenvalues. This observation—and the eigenspectrum of the modularity matrix in general—are, as we will see, closely tied to the community structure of the network.

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★ write \mathbf{s} as a linear combination of the normalized eigenvectors \mathbf{u}_i of the modularity matrix, $\mathbf{s} = \sum_{i=1}^n a_i \mathbf{u}_i$ with $a_i = \mathbf{u}_i^T \mathbf{s}$. Then

$$Q = \frac{1}{4m} \sum_i a_i^2 \beta_i, \tag{29}$$

where β_i is the eigenvalue of \mathbf{B} corresponding to the eigenvector \mathbf{u}_i . We now assume that the eigenvalues are labeled in *decreasing* order $\beta_1 \geq \beta_2 \geq \dots \geq \beta_n$ and the task of maximizing Q is one of choosing the quantities a_i^2 so as to place as much as possible of the weight in the sum (29) in the terms corresponding to the largest (most positive) eigenvalues.

to \mathbf{u}_1 . Again as before, however, good approximate solutions can be obtained by choosing \mathbf{s} to be as close to parallel with \mathbf{u}_1 as possible, which is achieved by setting

$$s_i = \begin{cases} +1 & \text{if } u_i^{(1)} \geq 0, \\ -1 & \text{if } u_i^{(1)} < 0. \end{cases} \tag{30}$$

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the elements of the eigenvector \mathbf{u}_1 also contain useful information about the network, indicating, as discussed in [32], the “strength” with which vertices belong to the communities in which they are placed

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Section IV B and C contain algorithms for dividing networks into more than 2 communities with implementation in Sections V and VI and VII.
[because] it is certain that repeated subdivision of a network into two parts will in some cases fail to find the optimal modularity configuration.