Spectral community detection in sparse networks

M. E. J. Newman
Department of Physics, University of Michigan, Ann Arbor, MI 48109 and Santa Fe Institute, 1399 Hyde Park Road, Santa Fe, NM 87501

Spectral methods based on the eigenvectors of matrices are widely used in the analysis of network data, particularly for community detection and graph partitioning. Standard methods based on the adjacency matrix and related matrices, however, break down for very sparse networks, which includes many networks of practical interest. As a solution to this problem it has been recently proposed that we focus instead on the spectrum of the non-backtracking matrix, an alternative matrix representation of a network that shows better behavior in the sparse limit. Inspired by this suggestion, we here make use of a relaxation method to derive a spectral community detection algorithm that works well even in the sparse regime where other methods break down. Interestingly, however, the matrix at the heart of the method, it turns out, is not exactly the non-backtracking matrix, but a variant of it with a somewhat different definition. We study the behavior of this variant matrix for both artificial and real-world networks and find it to have desirable properties, especially in the common case of networks with broad degree distributions, for which it appears to have a better behaved spectrum and eigenvectors than the original non-backtracking matrix.

Since their introduction in the 1970s, spectral methods for the analysis of large graphs and networks have become a mainstay in the study of empirical network data [1]. One represents the structure of the network of interest using any of several matrix forms such as the adjacency matrix or graph Laplacian, then inspects the eigenvalues and eigenvectors for information about network structure. Experiments show (and it can be proven for some model networks) that the eigenvalue spectrum typically consists of a dense “spectral band” of closely spaced eigenvalues akin to an allowed energy band in condensed matter, plus some number of outlying eigenvalues separated from the band by a significant band gap. The eigenvectors corresponding to these outliers contain information about the large-scale structure of the network and particularly about so-called community structure, divisions of the network into groups that are tightly knit internally but only loosely connected externally. Spectral methods are of particular interest because the eigenvectors can reveal large- or global-scale structure within networks, by contrast with most other methods of network analysis, which focus on local properties.

Spectral methods can fail, however. The primary mode of failure is one familiar in condensed matter physics, namely the occurrence of defects or Griffiths singularities. Rarely occurring but dense subgraphs within a network can give rise to additional eigenvalues outside the main spectral band, akin to Lifshitz tails, which can reduce or eliminate the spectral gap. The corresponding eigenvectors can mix with the vectors containing community information, introducing noise or, in extreme cases, rendering community detection impossible. The simplest example of this phenomenon is the occurrence of hubs in a network, vertices of unusually high degree, which produce outlying eigenvectors strongly localized around the hubs and lacking global structure [2, 3]. In networks where the average degree of most vertices is high—much greater than one—the effect of hubs is diluted and not usually a problem. But in very sparse networks, those with small average degree, the effect becomes strong and renders conventional spectral methods virtually useless in many cases. Unfortunately, many of the networks encountered in practical studies, including social, technological, and biological networks, fall into this sparse category. The average degree of the Internet, coarse-grained at the level of autonomous systems, for example, is about six [4]. The average degree of metabolic networks is similar [5]. A large list of networks given in [6] contains hardly any networks with mean degree greater than ten.

An interesting solution to these problems has been put forward recently by Krzakala et al. [7], who propose focusing on the eigenvalues and eigenvectors of a different matrix representation of network structure, which they call the non-backtracking matrix, also called the Hashimoto edge matrix by previous authors [8, 9]. They show that for certain model networks this matrix displays a nonzero spectral gap even when mean degree is very small, with outlying eigenvalues that are well separated from the main spectral band, and hence that the matrix avoids many of the problems that hamper other matrix representations in the sparse limit. Moreover, they give results, both analytic and numerical, showing that a simple clustering of the elements of the leading eigenvectors of the matrix is able to accurately detect community structure in their networks.

In the present paper we propose and study a variant of the non-backtracking matrix, which we call the flow matrix, that shares many of the advantages of the non-backtracking matrix, but also avoids some of its problems. Our study of the flow matrix is motivated by several observations. As we will show, the standard objective function known as modularity, widely used in optimization schemes for community detection, can be written straightforwardly in terms of the flow matrix,
and hence spectral methods based on the flow matrix are equivalent to approximate optimization of the modularity, providing a connection to established methods for the community detection problem. Furthermore, we present results showing that the spectrum of the flow matrix is in some respects better behaved than that of the original non-backtracking matrix, particularly for networks with broad degree distributions, which includes most real-world networks. In particular, by contrast with the non-backtracking matrix, the flow matrix preserves a clear band edge in such networks, and the elements of its leading eigenvectors are tightly peaked allowing for straightforward community identification and giving better results in some practical situations.

Consider an undirected network with \( n \) vertices and \( m \) edges, no multiedges or self-loops, and only a single component. For such a network the original non-backtracking matrix is defined as follows [7, 8]. One first converts the network into a directed network by replacing each undirected edge between a pair of vertices with two directed edges pointing in opposite directions between the same pair of vertices. Each of the \( 2m \) directed edges is given a label of the form \( i \rightarrow j \) indicating the vertex pair it connects and the direction in which it connects them. The non-backtracking matrix \( B \) is a \( 2m \times 2m \) non-symmetric matrix with one row and one column for each directed edge and elements

\[
B_{i \rightarrow j, k \rightarrow l} = \delta_{ij}(1 - \delta_{jk}),
\]

where \( \delta_{ij} \) is the Kronecker delta. In other words all elements are zero unless edge \( i \rightarrow j \) points out of the same vertex that edge \( k \rightarrow l \) points into, and edges \( i \rightarrow j \) and \( k \rightarrow l \) are not pointing in opposite directions between the same pair of vertices. Note that, since the non-backtracking matrix is not symmetric, its eigenvalues are in general complex, unlike those of most other matrix representations for undirected networks, but the largest eigenvalue is always real (by the Perron–Frobenius theorem) and in some cases there may be additional highly real eigenvalues as well.

The name “non-backtracking matrix” derives from a connection between the matrix and the properties of non-backtracking walks. A non-backtracking walk [9, 10] is a path across the edges of a network that is allowed to revisit a vertex visited previously but only after at least two other vertices have been visited; immediate revisits of the form \( 1 \rightarrow 2 \rightarrow 1 \) are prohibited. It is straightforward to show that powers of the non-backtracking matrix count non-backtracking walks and that traces of powers count closed non-backtracking walks. The spectrum of any matrix is given entirely by such traces of powers, via a derivative of the Stieltjes transform [12], and hence in this case by counts of closed non-backtracking walks.

Note that any subgraph of the network that takes the form of a tree, attached to the rest of the network at only a single point, contains no non-backtracking walks, since all such walks contain at least one loop and a tree contains none. Hence the presence (or absence) of such trees in the network has no effect on the spectrum and one can remove them. In the developments that follow we will assume that all such dangling trees have been removed, which will make our calculations simpler. A network with its dangling trees removed is called a 2-core. We will revisit the question of dangling trees in networks toward the end of this paper.

The primary result of Krzakala et al. [7] is that for certain classes of model networks the non-backtracking matrix has a sharp edge to its spectral band, with no Lifshitz tails, and a nonzero spectral gap, regardless of the average degree. It thus appears the matrix is immune to the problems that plague the Laplacian and other graph representations in the low-degree limit. Krzakala et al. give arguments indicating that the complex eigenvalues of the non-backtracking matrix for random graphs with Poisson degree distribution should lie with a circle of radius \( \sqrt{\langle d \rangle} \) in the complex plane, where \( \langle d \rangle \) is the mean degree of the graph, and in practice this result seems to work well on simulated networks. They also give a generalization to networks that have non-Poisson degrees, as most real-world networks do. For such networks the mean degree \( \langle d \rangle \) is replaced with the mean expansion rate of the network, which is \( \langle d^2 \rangle / \langle d \rangle - 1 \) for uncorrelated networks. This generalization, however, may be less useful in practical situations. In particular, in the common case of networks with power-law degree distributions the expansion rate diverges and with it the bound on the eigenvalues, and even for broad degree distributions with finite moments the bound may be very high.

In this paper we study a variant of the non-backtracking matrix which appears to be better behaved when networks have broad degree distributions, and which also has close connections to previously studied methods of community detection that are known to perform reliably under realistic circumstances. The matrix we study, which we call the flow matrix, is defined on the same \( 2m \) directed edges as the non-backtracking matrix, and has elements

\[
F_{i \rightarrow j, k \rightarrow l} = \frac{\delta_{ij}(1 - \delta_{jk})}{d_i - 1},
\]

where \( d_i \) is the degree of vertex \( i \). The flow matrix can be thought of as a conservative-flow version of the non-backtracking matrix that describes the motion of a conserved quantity around the network, but subject to a non-backtracking constraint. Its powers count non-backtracking walks weighted inversely by the product \( \prod (d_i - 1) \) for the vertices they traverse.

The flow matrix has a close connection to the standard objective function known as modularity, as we can show by the following argument. Given a network and a division of that network into communities or groups, the modularity \( Q \) is defined to be the fraction of edges
that fall within communities minus the expected value of
the same fraction if edges were placed at random [13]. In
mathematical terms,
\[ Q = \frac{1}{2m} \sum_{ij} \left[ A_{ij} - \frac{d_i d_j}{2m} \right] \delta_{g_i, g_j}, \tag{3} \]
where \( g_i \) is the label of the group to which vertex \( i \) belongs
and \( A_{ij} \) is an element of the adjacency matrix \( A \), having
value 1 if there is an edge between vertices \( i \) and \( j \) and
zero otherwise. The modularity quantifies how good our
division of the network is and modularity-based community
detection methods find good divisions by maximizing
it over divisions, i.e., over the group assignments \( g_i \).

Consider the simplest example of this maximization
problem, where the network is divided into just two
groups (of any size) and define a set of \( n \) index vari-
bles \( s_i \), one for each vertex, such that \( s_i = +1 \) if vertex \( i \)
belongs to group 1 and \(-1\) if it belongs to group 2. Then
consider the following scalar quadratic form involving the
flow matrix:
\[ R = u^T (F - 11^T) v, \tag{4} \]
where \( u \) and \( v \) are two \( 2m \)-element vectors that we choose
and \( 1 \) is the uniform unit vector \( 1 = (1, 1, 1, \ldots) / \sqrt{2m} \). If
we make the particular choice \( u_{i \rightarrow j} = v_{i \rightarrow j} = s_j \),
meaning that the elements of both vectors are equal to the
group index of the vertex to which the corresponding
edge points, then
\[
u^T F v = \sum_{\text{edges } i \rightarrow j} \frac{\delta_{ij}(1 - \delta_{jk})}{d_i - 1} s_j s_l
= \sum_i \frac{s_i}{d_i - 1} \sum_j A_{ij} A_{ki} (1 - \delta_{jk}) s_j
= \sum_i \frac{s_i}{d_i - 1} \sum_j (d_j - 1) A_{ij} s_j = s^T A s, \tag{5} \]
where \( s \) is the \( n \)-element vector with elements \( s_i \). Also
\[ u^T 11^T v = \frac{1}{2m} \sum_{\text{edges } i \rightarrow j} \sum_{k \rightarrow l} s_j s_l
= \frac{1}{2m} \sum_{ijkl} A_{ij} A_{kl} s_j s_l
= \frac{1}{2m} \sum_{j} d_j s_j s_l = s^T d d^T 2m s, \tag{6} \]
where \( d \) is the \( n \)-element vector with elements equal to
the degrees \( d_i \). Noticing that \( \frac{1}{2}(s_j s_j + 1) \) is 1 if \( i \) and \( j \)
are in the same group and zero otherwise, we can now
combine Eqs. \( 3 \), \( 5 \), and \( 6 \) to get an expression for the
modularity:
\[ Q = \frac{1}{4m} \sum_{ij} \left[ A_{ij} - \frac{d_i d_j}{2m} \right] (s_i s_j + 1) = \frac{1}{4m} s^T \left[ A - \frac{d d^T}{2m} \right] s
= \frac{1}{4m} u^T (F - 11^T) v = R, \tag{7} \]
where in the second equality we have made use of the
fact that \( \sum_{ij} A_{ij} = \sum_i d_i = 2m \).
In other words, \( R \) is simply equal to the modularity.
The goal of modularity-based community detection is to
find the group indices \( s_i \) that maximize the modu-
larility. This optimization is known, in general, to be a
hard computational problem [14], but good approximate
solutions can be found by a variety of heuristics. Here
we use a standard relaxation technique, in which we re-
xact the condition that the elements of \( u \) and \( v \) are equal
to \( s_i = \pm 1 \), allowing them to take any real values. We
must be careful, however—if the magnitudes of \( u \) and \( v \)
can become arbitrarily large then there is no limit on the
degree of the modularity. To prevent this happening
we impose an additional constraint. We note that when
\( u_{i \rightarrow j} = v_{i \rightarrow j} = s_j \) we have \( u^T v = 2m \), a constant,
and we will impose the same constraint on our relaxed
optimization. Clearly the original unrelaxed values of the
vector elements satisfy this constraint, so the relaxed
optimization includes these values, but it includes many
other values as well.

The maximization of Eq. \( 7 \) in this relaxed solution
space is straightforward. Introducing a Lagrange mul-
iplier \( \lambda \) to enforce the constraint on \( v \) and differen-
tiating with respect to the elements of \( u \), we find that the
maximum modularity occurs when
\[ (F - 11^T) v = \lambda v. \tag{8} \]
In other words \( v \) is an eigenvector of the matrix \( F - 11^T \)
with eigenvalue \( \lambda \). Substituting this solution back into
Eq. \( 7 \) then gives
\[ Q = \frac{1}{4m} u^T (F - 11^T) v = \frac{\lambda}{4m} u^T v = \frac{\lambda}{2}. \tag{9} \]
Thus the maximum modularity is given by setting \( v \)
equal to the eigenvector for the largest (most positive)
eigenvalue of the matrix.

This constitutes an exact solution of the relaxed max-
imization problem, which we now use as a guide to the
solution of the original unrelaxed problem of finding the
quantities \( s_i = \pm 1 \) on the vertices. Recalling that in the
unrelaxed formulation all vector elements \( v_{i \rightarrow j} \) are equal
to \( s_j \), we see that our relaxed solution for \( v \) in fact gives
us \( d_j \) different values for \( s_j \), one for every edge incident
on \( j \). We estimate the true \( s_j \) by taking the average of
these values and rounding to the nearest \( \pm 1 \), which in
practice means \( s_j = +1 \) if the sum \( \sum_i A_{ij} v_{i \rightarrow j} \) is positive
and \( s_j = -1 \) if the sum is negative.

Thus our spectral algorithm is a simple one: we calcu-
late the leading eigenvector of the matrix \( F - 11^T \),
sum the elements pointing to each vertex, and divide the
vertices into two groups according to the signs of these
sums. This is essentially the algorithm used by Krza-
akal et al. in their calculations except that we use the
normalized version of the non-backtracking matrix—the
flow matrix—rather than the original non-backtracking matrix. As with all relaxation methods, this one gives only an approximation to the true optimum of our objective function, but as we will see it performs well in practice.

We observe the following about the eigenvectors of the matrix $F$. The $i \to j$ row of the matrix contains $d_i - 1$ nonzero elements with value $1/(d_i-1)$ each, meaning that the uniform vector $\mathbf{1}$ is a (properly normalized) eigenvector of the matrix with eigenvalue 1. Thus it is also an eigenvector of $F - 11^T$, but with eigenvalue zero. All other eigenvalues and eigenvectors of $F - 11^T$ are the same as those for $F$. By the Perron–Frobenius theorem the vector $\mathbf{1}$ is the leading eigenvector of $F$ (since it has all elements positive and the network is connected), while for the matrix $F - 11^T$, which has this eigenvector removed, the most positive eigenvalue must equal the second eigenvalue of $F$ (so long as $F - 11^T$ has any positive eigenvalues). Thus we can, as we wish, perform community detection using either the leading eigenvector of $F - 11^T$ or the second eigenvector of $F$. The results will be identical. In this paper we do the latter, since it is slightly simpler in practice.

We have performed a number of numerical calculations of the spectrum of the flow matrix, along with tests of the community detection algorithm derived above. Figure 1 shows results for (the largest 2-core of) a computer-generated network created using the degree-corrected block model of [12] with two communities. This model allows one to generate networks that simultaneously contain planted community structure and nontrivial degree distribution. In our tests we generated networks with a power-law degree distribution with exponent $-2.5$ to test the behavior of our methods in the case of realistically high degree variance. The top left panel of Fig. 1 shows the spectrum of the flow matrix in the complex plane for a network of $n = 1000$ vertices. As the figure shows, the eigenvalues fall neatly within a circular region with a clear band edge and there are two outlying eigenvalues. An argument analogous to that of [17] indicates that the eigenvalues lie within a circle of radius \( \sqrt{d/(d-1)} \langle d \rangle \), which is never greater than 1. Such a circle is plotted in Fig. 1 and appears to agree well with the numerical results.

Of the two outlying eigenvalues, the higher one has value 1 and eigenvector $\mathbf{1}$ as we have said; the lower one contains the community structure. The center left panel shows our relaxed estimates of the group membership variables $s_i$ from the second eigenvector, and the two planted groups in the network (of equal sizes in this case) are clearly visible. Dividing the vertices according to the signs classifies 93% of them into the correct groups. Apart from modest statistical fluctuations, these results appear robust over repetitions of the experiment with the same parameters. The bottom left panel of the figure shows the distribution of the eigenvector elements for the flow matrix, with two clear peaks that correspond closely to the planted communities in the network.

For comparison we show in the right three panels of the figure the corresponding quantities for the original non-backtracking matrix. The non-backtracking matrix also does a good job of classifying vertices into groups, with only a modestly lower fraction 90% of vertices classified correctly. The spectrum of the matrix is less well behaved, however. As the top right panel shows, the spectrum is more diffuse than that of the flow matrix, having no clear circular edge. And while there are still two outlying eigenvalues, the estimates of $s_i$ calculated from the second eigenvector, shown in the center right panel, are noisier, with a strongly non-Gaussian distribution and occasional large fluctuations. Similar fluctuations are also seen in, for example, spectra of the or-
Flow
Non-backtracking

Before closing, let us return to an issue raised at the start of this paper, that of dangling trees attached to a network. The original non-backtracking matrix takes no account of such trees—when they are removed, leaving the 2-core of the network, both the eigenvalues and eigenvectors of the matrix are unchanged (within the 2-core) from those of the full network. This is perhaps the most serious drawback of the method as proposed—widely used and trusted methods of community detection, such as modularity maximization or inference methods based on block models, can give very different answers for networks with and without dangling trees, and hence can disagree strongly with methods based on the non-backtracking matrix. The variant matrix discussed here to some extent remedies this problem: its spectrum does change when dangling trees are added to or removed from the network, and one can write a version of Eq. (7) that is correct for all networks, not just those consisting of a 2-core, so that relaxations give an approximation to the maximum modularity partitioning of any network. The problem is not completely solved, however, as one can see by considering the extreme case of a network composed of a single tree with no 2-core at all. Because the spectra of both the matrices $B$ and $F$ are determined by counts of non-backtracking walks, and because there are no such walks on a tree, all eigenvalues of both matrices are zero and the eigenvectors fail to give any partition for such a network, even though other methods, including exact modularity maximization, give sensible partitions when applied to trees. It is an open question whether and how this problem can be remedied.

The author thanks Tammy Kolda, Cris Moore, Elchanan Mossel, Joe Neeman, and Lenka Zdeborová for useful conversations. This work was funded in part by the National Science Foundation under grant DMS–1107796 and by the Air Force Office of Scientific Research (AFOSR) and the Defense Advanced Research Projects Agency (DARPA) under grant FA9550–12–1–0432.

[1] U. von Luxburg, A tutorial on spectral clustering. *Statistics and Computing* **17**, 395–416 (2007).
[2] K.-I. Goh, B. Kahng, and D. Kim, Spectra and eigenvectors of scale-free networks. *Phys. Rev. E* **64**, 051903 (2001).
[3] R. R. Nadakuditi and M. E. J. Newman, Spectra of random graphs with arbitrary expected degrees. *Phys. Rev. E* **87**, 012803 (2013).
[4] M. Faloutsos, P. Faloutsos, and C. Faloutsos, On power-law relationships of the internet topology. *Computer Communications Review* **29**, 251–262 (1999).
[5] H. Jeong, B. Tombor, R. Albert, Z. N. Oltvai, and A.-L. Barabási, The large-scale organization of metabolic networks. *Nature* **407**, 651–654 (2000).
[6] M. E. J. Newman, *Networks: An Introduction*. Oxford University Press, Oxford (2010).
[7] F. Krzakala, C. Moore, E. Mossel, J. Neeman, A. Sly, L. Zdeborová, and P. Zhang, Spectral redemption: Clustering sparse networks. Preprint arXiv:1306.5550 (2013).

[8] K. Hashimoto, Zeta functions of finite graphs and representations of p-adic groups. Adv. Stud. Pure Math. 15, 211–280 (1989).

[9] O. Angel, J. Friedman, and S. Hoory, The non-backtracking spectrum of the universal cover of a graph. Preprint arXiv:0712.0192 (2007).

[10] N. Alon, I. Benjamini, E. Lubetzky, and S. Sodin, Non-backtracking random walks mix faster. Communications in Contemporary Mathematics 9, 585–603 (2007).

[11] R. Fitzner and R. van der Hofstad, Non-backtracking random walk. J. Stat. Phys. 150, 264–284 (2013).

[12] T. Tao, Topics in Random Matrix Theory. American Mathematical Society, Providence, RI (2012).

[13] M. E. J. Newman and M. Girvan, Finding and evaluating community structure in networks. Phys. Rev. E 69, 026113 (2004).

[14] U. Brandes, D. Delling, M. Gaertler, R. Görke, M. Hoefer, Z. Nikoloski, and D. Wagner, On finding graph clusterings with maximum modularity. In Proceedings of the 33rd International Workshop on Graph-Theoretic Concepts in Computer Science (2007).

[15] B. Karrer and M. E. J. Newman, Stochastic blockmodels and community structure in networks. Phys. Rev. E 83, 016107 (2011).

[16] D. Lusseau, K. Schneider, O. J. Boisseau, P. Haase, E. Slooten, and S. M. Dawson, The bottlenose dolphin community of Doubtful Sound features a large proportion of long-lasting associations. Behavioral Ecology and Sociobiology 54, 396–405 (2003).