Identifying overlapping communities as well as hubs and outliers via nonnegative matrix factorization

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Community detection is important for understanding networks. Previous studies observed that communities are not necessarily disjoint and might overlap. It is also agreed that some outlier vertices participate in no community, and some hubs in a community might take more important roles than others. Each of these facts has been independently addressed in previous work. But there is no algorithm, to our knowledge, that can identify these three structures altogether. To overcome this limitation, we propose a novel model where vertices are measured by their centrality in communities, and define the identification of overlapping communities, hubs, and outliers as an optimization problem, calculated by nonnegative matrix factorization. We test this method on various real networks, and compare it with several competing algorithms. The experimental results not only demonstrate its ability of identifying overlapping communities, hubs, and outliers, but also validate its superior performance in terms of clustering quality.
have not been included in any of them are outliers. In summary, CDNMF is capable of identifying overlapping communities as well as detecting hubs and outliers simultaneously.

The nature of the problem incurs a plethora of work in literature, and we only mention some new results that closely relate to us. For example, Xu et al. introduced a method called SCAN which detects communities with overlapping vertices (which they called hubs) and outliers in the network. Berton introduced a distance measure using random walk, and then introduced the dissimilarity index between pairs of vertices based on it. By ranking the dissimilarity index, outliers could be detected. But this method just focuses on finding the outliers, while it does not consider the detection of communities. However, it considers hubs as outliers, which seems to be unreasonable. Zhao et al. considered that many networks contain vertices that do not fit in with any of the communities, and thus forcing all vertices into communities could distort the results. They extracted the cores of the networks and allowed for arbitrary structure in the remainder of the network, which could include weakly connected vertices, as the “background.” But they defined most of the vertex in a network as outliers, which was too sweeping to be compared with the traditional definition of outliers. Chen and Saad held the opinion that not every participating vertex in the network needed to belong to a community as before, and they proposed a method to extract meaningful dense subgraphs from given networks. However, they extracted dense subgraphs regardless of the rest vertices, and still their method does not have the capability to detect hubs.

Nonnegative Matrix Factorization (NMF) is a feature extraction and dimensionality reduction technique in machine learning, which has been adapted to community detection recently. For example, Zarei et al. presented a NMF-based algorithm for identifying fuzzy communities, where the new feature matrix, called the vertex-vertex correlation matrix was introduced. Psorakis et al. presented an approach to community detection that utilizes a Bayesian nonnegative matrix factorization model to extract soft modules from networks. Wang et al. proposed a symmetric NMF technique to detect overlapping communities in networks. Zhang and Yeung proposed a community detection method called BNMTF, which is based on the bounded nonnegative matrix factorization. Using three factors in the factorization, they could explicitly model and learn the community membership of each vertex. However, the current NMF-based methods only focuses on the detection of communities, but none of them take into account the identification of vertex roles, such as hubs and outliers.

Also of note is several related works which adopts similar models. But rather than using loss function, they adopts the likelihood probability as the goal, and take a different algorithmic approach such as expectation-maximization algorithm to learn the model. Still, as with the above NMF-based methods, they only considers the detection of communities, and does not refer to the hubs or outliers.

Results
In this section, we demonstrate the effectiveness of our method CDNMF at exploring the three kinds of vertex roles by applying it on some real-world datasets. The experimental results verify that CDNMF can reveal rich information on these networks.

Real world networks examples. The School Friendship Network was compiled from the National Longitudinal Study of Adolescent Health. It is based on self-reporting from students, which are from different grades, from grade 7 to grade 12. But in grade 9, there are two subgraphs, which correspond to the groups of white and black students, respectively.

By setting the group number \( K = 6 \), we fit our model to the school friendship network data. Figure 1 shows our community result, which roughly matches the ground-truths of this network. The hubs

Figure 1 | Our community result. Here different shapes represent the real community membership, and different colors represent different communities detected (except pink vertices). The hubs are marked by black boxes, such as vertices 15 and 35; the overlapping vertices are shown as pie vertices, such as vertices 45 and 46; and the rest vertices, colored by pink, are outliers, such as vertices 25 and 42.
are drawn larger (in black boxes), and they all have strong links to other students in their communities. The overlapping vertices are those students who have many relations in different communities, which imply that they communicate with these communities frequently, although they still mainly belong to the grades where they are in the ground-truths. What’s more, the distribution of overlapping students often lies between the adjacent grades. This phenomenon is very sensible in the reality where students in the adjacent grades often communicate more frequently than that in non-adjacent grades. Besides, Xie et al. posed a problem that some vertices (such as vertex 42) serve as a bridge between groups but do not have particular coherence to any group, and it is still not clear whether these vertices are really meaningful or necessary to be considered as “overlapping.” Here we give the answer. In our result, we consider vertices 42, 58, and 60 as outliers, and find that there are key differences between these vertices and the overlapping ones. They all have weak links to different communities, implying their relations with students either in their grades or in other grades are weak. This is a different behavior from the overlapping students, which implies these outliers are not as “gregarious” as the overlapping ones. Hence maybe they should be given more care about. Therefore, we believe it has more sense to assign such “bridge” vertices as outliers. Obviously, the identification of these three types of roles reveals more important and interesting information, and gives us a better understanding of this network.

The Dolphins Social Network was reported by Lusseau. In this network, dolphins represented as vertices have a link with each other if they are observed together more often than expected by chance over a period of seven years from 1994 to 2001. It is mainly divided into the male dolphins and female dolphins, which are marked by the cycle vertices and square vertices, respectively (see Figure 2).

By setting the group number $K = 2$, we fit our model to the dolphins social network data. Our community result has been shown in Figure 2 with different colors. As we can see, “sn100” is an overlapping vertex lying between the two communities and has some links to both of them; it is thus not proper to assign it to only one community. Besides, this vertex has the highest value of betweenness, leading to the fission of the dolphin community of doubtful sound into subgroups, which is clearly playing an important role holding the network together. Notice that the betweenness is a measure of the influence of individuals in a network over the flow of information between others, which makes sense to consider it as an overlapping vertex of the two communities. Moreover, our method successfully finds the outliers, such as “zig,” “snm5,” “pl,” most of which possess a same behaviour that just have one or two links with each community. Especially, “pl” belongs to the male community in the reality but has more links with the female community, thus some other community detection methods often misclassified it to be a female dolphin. Differently, our method neither misclassifies it to the female community nor assigns it to the male community, but considers it as an outlier. This assignment provides a new insight and involves deeper understanding for this network.

The Political Books Network was compiled by Valdis Krebs. This network represents books about US politics sold by Amazon.com. Edges represent frequent co-purchasing of books by the same buyers, as indicated by the “customers who bought this book also bought these other books” feature on Amazon. The political viewpoints of these books are given by “liberal,” “neutral” and “conservative,” respectively, which are taken as the ground-truth in our experiment.

By setting the group number $K = 3$, we fit our model to the political books network data. Our community result is shown as Figure 3. Because the topological structure of the “neutral” community is not clear, it’s a common challenge for most community detection algorithms. Here, our method successfully finds the domains of “conservative,” “neutral” and “liberal,” respectively. For instance, vertex “Why America Slept” is an overlapping vertex between “conservative” and “neutral,” which means it is often co-purchased by the same buyer. Although it is marked by “neutral,” we infer that it may contain both of the two viewpoints but mainly belongs to “neutral” part. More interestingly, the overlapping vertices are all between “conservative” and “neutral,” or between “liberal” and “neutral,” but not between “conservative” and “neutral.” It makes sense that the same buyer seldom buys two books with the clearly opposite political views, but has some probability to choose two books with similar or relative soft views. In addition, we find the hubs “A National Party No More” and “Bushwhacked” in the “conservative” and “liberal” communities, respectively. We guess these two books may be very popular in the two communities, which is correctly the situation in the reality. Considering the detected outliers, most of them locate at the borderline in the network. It implies they have weak links to other vertices, and probably are not as popular as other books in each community. In summary, our method can not only detect the community structure, but also provide some more useful information for this network.

**Figure 2** | Our community result for the dolphin social network. Here different shapes represent the real community membership, and different colors represent different communities detected (except pink vertices). The hubs (vertices “Web” and “Grin”) are shown in the black boxes; the overlapping vertex “SN100” is shown by pie vertex; and the rest, colored by pink, such as vertices “Zig,” are outliers.
The Karate Club Network\(^2\) has become a *de facto* testbed for community detection algorithms. A disagreement developed between the administrator (vertex 33) of the club and the club’s instructor (vertex 1), which ultimately resulted in the instructor’s leave and starting a new club. These two groups are used as the ground-truth in our study.

By setting the group number $K = 2$, we fit our model to the karate club network data. Our community result is shown in Figure 4, which roughly corresponds to the actual communities of this network. Especially, vertices 1, 33, and 34 are hubs found by CDNMF, vertices 3, 9, 31, and 32 are overlapping vertices, and vertex 17 is an outlier. In fact, vertex 17 locates at the borderline position of the left community, and it only connects the other two unimportant vertices 6 and 7, which causes it has only weak association with this community, and thus it is considered as an outlier vertex. Differently, vertex 12 has only one link with this community, but it connects with the club’s instructor (vertex 1) directly, which means it may be as well as an important vertex. For this reason, it should not be found as an outlier vertex but a community vertex, which is correctly the result of our method. Our method successfully finds the overlapping communities, the hubs, and outlier simultaneously. Therefore, it can be regarded as a helpful supplement to vertex divisions by introducing some more information from the identification of vertex roles.

**Result comparisons.** Here we use CDNMF on ten widely used real-world networks, and compare it with several well-known community detection methods. The networks used are shown in table 1, where $n$ and $m$ denotes the numbers of vertices and edges, respectively, and $K$ denotes the actual number of communities in the network. Note that, “Friendship6” and “Friendship7” denote the same network, but they used different ground-truths; the last two networks “Jazz” and “Neural” do not have known communities. The methods compared include: Louvain method\(^22\) which is regarded as one of the best for vertex partition, CPM (Clique Percolation Method)\(^1\) which is the most prominent algorithm for overlapping community detection, and BNMF\(^8\)
and BNMTF\textsuperscript{26} which both are community detection methods based on NMF. In order to sufficiently evaluate the performance of different algorithms, we adopt two sets of comparisons in terms of accuracy and community quality, respectively.

**Accuracy comparisons.** There are various standard measures that can be used to compare the known community structure and the one delivered by the algorithm. CDNMF does not force every vertex into a community, and some of them are detected as outliers. This situation appears for CPM algorithm in like manner. Thus, for fair comparison, we choose the widely-used FVCC, which measures the fraction of vertices classified correctly\textsuperscript{18}, as the accuracy metric here. Table 2 shows the results of different algorithms in terms of accuracy and community quality, respectively.

Table 2 | Comparing CDNMF with Louvain, CPM, BNMF, BNMTF, and CDNMF on seven real-world networks in terms of FVCC

| Dataset     | Louvain | CPM  | BNMF | BNMTF | CDNMF |
|-------------|---------|------|------|-------|-------|
| Karate      | 97.06   | 75.00| 82.35| 52.94 | 100   |
| Dolphins    | 96.77   | 100  | 83.23| 67.74 | 98.11 |
| Friendship6 | 92.75   | 82.35| 86.39| 26.09 | 96.55 |
| Friendship7 | 91.30   | 82.35| 85.22| 36.23 | 94.74 |
| Polblogs    | 84.76   | 88.57| 81.52| 79.05 | 84.54 |
| Word        | 58.93   | 62.16| 55.36| 72.32 | 59.02 |
| Polblogs    | 96.17   | ---- | 93.15| 88.72 | 97.50 |

In the following, we will offer two types of comparisons for each network. The first one is with CPM\textsuperscript{3}, which is the most prominent algorithm for overlapping community detection. CPM takes some vertices of the network as background and does not classify them into any community. For fairness, when comparing with it, we take the subgraph processed by CPM as the targeted network. But the drawback of this comparison is that, it is on a subgraph rather than on a whole network. For this reason, we offer the second type of comparison with Louvain\textsuperscript{22}, which is regarded as one of the best algorithm for vertex partition by\textsuperscript{29}. In these two comparisons, we use the number $K$ of communities got by CPM and Louvain respectively as the quality metric. Different from the networks used before, these two ones considered here possess rich metadata which describe the structural and functional roles of each vertex. Therefore, we can evaluate the performance of different methods by measuring how well the discovered community structures reflect the metadata, which seems to be more convincing than using quality metrics designed only based on network topology.

Applications. We use our method CDNMF on two applications in biology science and cognitive psychology respectively, which are the molecular-biological network of protein-protein interactions and the network of word associations, to show its superior performance over the existing methods in solving real-world problems. Different from the networks used before, these two ones considered here possess rich metadata which describe the structural and functional roles of each vertex. Therefore, we can evaluate the performance of different methods by measuring how well the discovered community structures reflect the metadata, which seems to be more convincing than using quality metrics designed only based on network topology.

Protein-protein interaction network. In the first application, we considered a protein-protein interaction (PPI) network from *Saccharomyces cerevisiae*\textsuperscript{27}. It contains 2,640 vertices and 6,600 links, where vertices represent proteins and links denote pairwise physical interactions in the yeast.

For this network, we use the Gene Ontology (GO) terms\textsuperscript{30}, which are the most elaborate protein annotations available, as its metadata. It provides controlled vocabulary (GO terms) which describes certain aspects of protein characteristics (function, location, etc). Here we measured the quality of detected community structure by utilizing GO term enrichment analysis, which finds common biological meaning (i.e., significant shared GO terms) for the proteins within each community. Enrichment is computed using hyper-geometric test\textsuperscript{14}, and each shared GO term was assigned a $p$-value to quantify the significance of gene-term enrichment. For the quantitative evaluation of community structure quality, we used the average of numbers of significantly enriched GO terms (i.e., GO terms with $p$-value less than a threshold) for all communities as quality metric. Different thresholds for significance of gene-term enrichment may lead different results. For fairness, we set 10 different thresholds for the significance test.
The comparison of our method and CPM is shown in Figure 5(a). For seven in ten thresholds, communities attained by CDNMF always get much more enriched GO terms than that of CPM, which means our communities can better reflect the metadata. Of note, our method is run on the subgraph sifted by CPM, and the filtered network is more suitable for CPM than the original one, which makes this comparison partial to CPM. In this sense, our method still gets more significant communities. Thus, it can better show the superiority of our method over CPM.

Furthermore, the comparison of our method and Louvain is shown in Figure 5(b). It shows that our result is always better than that of Louvain as the threshold for the significance test is varied, which indicates it has better community results from the perspective of semantic analysis.

Word association network. The network analyzed here comes from the word associations, which is constructed from the University of South Florida Free Association Norms data set in the manner of. This network contains 5,017 vertices and 29,148 links, where each vertex represents a word, and each link between two words indicates that people always associated one endpoint of the link with its other one.

For this network, we use the WordNet database, which is built for semantic analysis, as the metadata. This database assigned a set of meanings/definitions or senses to each word (known as Synsets). We define a pair of words to be similar when they belong to a same Synset. To assess the quality of detected community structure, we compute the enrichment of vertex pair similarity. Particularly, enrichment is the average metadata similarity between all pairs of vertices that share a community, divided by the average metadata similarity between all pairs of vertices. The larger the enrichment, the better the community structure is.

First, we compare our method with CPM. The enrichment of our result is 51.28, which is much larger than that of CPM (30.75). It indicates that, even in the case of using CPM’s subgraph, the community result got by our method is still more reasonable than that of CPM in terms of real semantic. Thereafter, we compare our method with Louvain on the whole network. The enrichment of our result is 17.77, which is larger than that of Louvain (15.97). This result shows that, when compared with Louvain, our method can always get the better community result from the perspective of semantic analysis.

Discussion

In this work, we have proposed a novel method CDNMF based on NMF. Compared to previous work on roles identification of vertices in networks, CDNMF uses the centrality representation of vertices in each community, which enables us to identify not only all communities, but the different roles of vertices in the same run, including hubs and outliers. In contrast to other NMF-based methods, CDNMF avoids an artificial threshold in the detection of overlapping communities, which makes it much easier to implement. The experiments on various real-world networks, clearly demonstrated the superior performance of our method. We would like to draw attention to some information that are detected by CDNMF and possibly useful but missed by other algorithms that were applied on the same data sets.

Let us also point out some possible improvements to our method. In the current method, the number K of communities has to be predefined. This is not unique to our method, but commonly observed in all similar model-based methods. To surmount this obstacle, several methods have been proposed in literature, e.g., the minimum description length principle and multi-objective optimization, neither of which, however, is compatible with our framework or can be adapted in a natural way. We leave it open for the future work.
Model learning. Our task here is to learn the model mentioned before. We first define it as an optimization problem, and then infer the parameters by best fitting the observed network and the model specified in (4).

We use squared loss to measure the relaxation error. The loss function can be then formulated as

$$\min_{U,H} L(A, U, H) = \|A - \hat{A}\|^2_F$$

subject to

$$I_1^2 U = I_1^2,$$

$$H = \text{diag}(w^T) \text{, and}$$

$$w^T = (w_1, w_2, ..., w_n).$$

As $H$ is a diagonal matrix, the expected adjacency matrix $\hat{A}$ can be rewritten as

$$\hat{A} = UH^{1/2}U^T = (UH^{1/2})(UH^{1/2})^T = XX^T.$$  

(6)

Then, we can transform the optimization problem of (5) to be an equivalent problem of nonnegative matrix factorization:

$$\min_{X,U} \|A - XX^T\|^2_F.$$  

(7)

According to\(^7\), by using gradient descent method, we obtain the multiplicative updating rule of NMF style for the element $X_{ij}$ in $X$:

$$X_{ij} \propto X_{ij} \frac{(AX)_{ij}}{\sum_{k=1}^{n}(AX)_{ik}^2}.$$  

(8)

Now, the optimization of (7) is to iteratively solve (8) by choosing a set of initial values. When it converges, we can infer the model parameters using X. Using (6), we can obtain the degree matrix of communities by

$$H = (1)^T X,$$

(9)

and we then get the centrality matrix $U$ of vertices by

$$U = X(H^{1/2})^{-1}.$$  

(10)

Identifying overlapping communities, hubs, and outliers. When having the centrality matrix $U$ of vertices and the degree matrix $H$ of communities, here we introduce a method for detecting the overlapping communities, hub vertices, and outlier vertices.

As each column of $U$ denotes the centralities of all vertices in this community, we rank all the vertices in each column according to their values in decreasing order. For any community $\mathbf{z}$, the $\mathbf{z}$th column of ordered $U$ is denoted by $\hat{U}_{\mathbf{z}}$:

$$\hat{U}_\mathbf{z} = \left(\hat{u}_1^\mathbf{z}, \hat{u}_2^\mathbf{z}, ..., \hat{u}_n^\mathbf{z}\right)_C,$$

(11)

where $\hat{u}_i^\mathbf{z} \geq \hat{u}_i^\mathbf{z} \geq ... \geq \hat{u}_i^\mathbf{z} \geq ... \geq \hat{u}_n^\mathbf{z}$ and $1 \leq i \leq n$. Obviously, the upper the vertex, the more important it is in this community. The corresponding vertex vector of $\hat{U}_\mathbf{z}$ is denoted by $\hat{l}_\mathbf{z}$:

$$\hat{l}_\mathbf{z} = (l_1^\mathbf{z}, l_2^\mathbf{z}, ..., l_n^\mathbf{z}),$$

(12)

where $1 \leq j \leq n$, and $l_j^\mathbf{z}$ represents the vertex index corresponding to the value $\hat{u}_j^\mathbf{z}$.

From $H$, we get the expected degree of the $j$th community $w_j$. Then we add the vertex in $\mathbf{I}$ one by one from top to bottom to this community, until the sum of degrees of these vertices is larger than $w_j$. The real degree of community $\mathbf{z}$ is then evaluated by

$$\hat{d}_\mathbf{z} = \sum_{j=1}^{n} A_{j\mathbf{z}} \hat{l}_j,$$

(13)

where $p$ indicates that number of vertices having been added in the $j$th community.

Then the members of the $\mathbf{z}$th community $C_{\mathbf{z}}$ is:

$$C_{\mathbf{z}} = \left\{ l_j^\mathbf{z} \mid 1 \leq j \leq p, ~ \text{if} ~ |D_{\mathbf{z}} - w_j| \leq |D_{\mathbf{z}} - w_{j-1}| \right\} \cup \left\{ l_j^\mathbf{z} \mid 1 \leq j \leq p-1, ~ \text{if} ~ |D_{\mathbf{z}} - w_j| > |D_{\mathbf{z}} - w_{j-1}| \right\}.$$  

(14)

As we can see, these communities will overlap with each other when they are overlapping in nature. We then get the overlapping communities.

After getting all the communities, the outliers set $O$ in the network can be then calculated as:

$$O = V - \bigcup_{z=1}^{K} C_{\mathbf{z}},$$

(15)

and the hubs set $B$ is evaluated as:

$$B = \{ l_{j}^\mathbf{z} \mid 1 \leq j \leq K \}.$$  

(16)

In this way, if a vertex is a hub, it is ranked in the top in the column, sequentially, it can be easily detected. If a vertex is an outlier, it is ranked below the cut position, i.e., it links to other communities via weak relations. If a vertex resides in the overlapping region of communities $\mathbf{r}$ and $\mathbf{s}$, it will have high centrality in both these two communities and be added to them simultaneously. In addition, in some particular applications, we may consider the first two vertices as the hubs, such as the two leaders in the cycle community in the karate network (see Figure 4). Moreover, different from other models\(^8\)\(^\text{--}^{14}\), which need the specified threshold to detect overlapping communities, our CDNMF can detect three types of vertex roles including overlapping communities without any threshold.

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**Author contributions**

X.C., X.W., D.J. and Y.C. designed the research; X.W., D.J. and D.H. performed the research, analyzed the data and prepared the figures and tables; all authors reviewed the manuscript.

**Additional information**

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