Identifying clusters of vertices in graphs continues to be an important problem and modularity continues to be used as a tool for solving the problem. Modularity, which measures the quality of a division of the vertices into clusters, explicitly treats vertices of different degrees differently, imposing a larger penalty when high-degree vertices are put in the same cluster. We claim that this unequal treatment negatively impacts the performance of clustering algorithms based on modularity for graphs with heavy-tailed degree distributions. We used the Greedy Modularity hill-climb to find clusters in graphs with power-law degree distributions and observed that it performed poorly clustering low-degree vertices. We propose a simple variant of modularity that we call flat modularity. We found that using the same algorithm with the modified score instead improved the performance of the clustering algorithm on low-degree vertices and overall as well. We believe that changing to flat modularity, which should also simplify implementations, could improve clustering performance in the many real-world processes that rely on modularity.

1. Introduction

Finding communities in graphs continues to be an important problem. Many algorithms for doing so rely on modularity as the measure of the quality of the clustering. Modularity is known to have drawbacks and other quality measures have been proposed. Despite this, modularity continues to be used and there is continued value in improving our understanding of the metric. Many graphs have degree distributions with a heavy tail. Whether these arise from a power-law or some other distribution, these graphs have some vertices with very large degree and many vertices with a low degree. Modularity explicitly treats vertices of different degrees differently, imposing a larger penalty when high-degree vertices are put in the same cluster. We posit that clustering algorithms that use modularity as the score will perform poorly on lower-degree vertices.

We propose a natural variant of modularity, flat modularity, which does not differentiate between the vertices based on their degrees. We use the Greedy Modularity algorithm to cluster using modularity and also with our proposed modularity variant on LFR graphs that have degree distributions satisfying a power law. We compare the resulting clusters to the planted clusters and evaluate the results using the Matthews correlation coefficient. We observe that climbing using our variant score improves the match to the planted clusters. We also observe that the gain in performance seems to come by improving the clustering of low-degree vertices, see Figure 3 on page 5.
2. Modularity

Given a division of the vertices of a graph into clusters, modularity compares the fraction of edges internal to clusters to the average value over all graphs with the same degree distribution (where we allow multiple edges and loops). One of the many ways to write the modularity of a given division into clusters is

\[
Q = \frac{1}{2L} \sum_v \sum_w C_{vw} \left( A_{vw} - \frac{k_v k_w}{2L} \right)
\]

where \(Q\) is the modularity, \(L\) the number of edges in the graph, \(k_v\) the degree of the vertex \(v\), and \(A\) and \(C\) are adjacency matrices, \(A\) for the graph and \(C\) for the clusters; that is \(C_{vw} = 1\) when \(v\) and \(w\) are in the same cluster and \(C_{vw} = 0\) otherwise.

We interpret modularity as containing a bonus \(A_{vw}\) for putting adjacent vertices into the same cluster. The penalty \(k_v k_w/(2L)\) encourages keeping vertices separate. This penalty therefore varies among the pairs of vertices and our primary question is whether or not this is desirable.

Modularity is the main ingredient in a number of algorithms intended to divide the vertices of a graph into clusters. We will use the Greedy Modularity algorithm [7] though the Louvain algorithm [3] is known to have a better run-time. A more recent example can be found in [8]. Algorithms based on modularity continue to be used to identify clusterings [4]. We chose Greedy Modularity because it is a simple climb and we believe that this places more weight on the score being used than a more complex climb.

It is now known [9] that modularity has a fundamental drawback, called the resolution limit. Modularity tends to want to collapse clusters that are smaller than this resolution limit. A common workaround is to add a resolution \(r\) to the modularity, forming

\[
Q_r = \frac{1}{2L} \sum_v \sum_w C_{vw} \left( r \cdot A_{vw} - \frac{k_v k_w}{2L} \right)
\]

for a value \(r\) between 0 and 1; we reduce the reward for putting adjacent vertices into the same cluster. This increases the relative effect of the penalty and hence discourages combining communities.

A large number of other measures of the quality of a division into clusters have been proposed. Many are considered in [17] which also suggests different ways to evaluate these measures. We are going to use artifical graphs with planted clusters and that simplifies the evaluation phase.

3. Some power-law graphs

The penalty term in the formula for modularity, \(\frac{k_v k_w}{2L}\), explicitly depends on the degrees of the vertices. In many real world graphs, for example those arising from power grids or cell interconnections, geometry forces all vertices to have degrees in a relatively small range. In this case, having the penalty depend on the degree will have only a minor effect. Other real world graphs, for example those arising from web page links or social networks, the degree distribution can be quite heavy-tailed (see [2] for further discussion). In this case, the magnitude of the penalty can cover a large range.
To study the consequences of the widely varying penalty, we will use LFR graphs, [12]. Specifically, we use the implementation of these graphs in the NetworkX [10] function \texttt{LFR\_benchmark\_graph}. We will use \texttt{gamma} (that is, \(\gamma\)) for the exponent in the power law of the degree distribution and vary a random seed \texttt{seed} as we construct the graph. All of the other parameters are specified in Figure 1. While one of our inputs seems to say that the maximum degree will be 50, in fact our graphs commonly have higher degrees. For one example we looked at, the degrees ran from 14 to 67. The input parameter with value 1000 represents the number of vertices in the graph. The input parameter with value 2 is the exponent in a power law for the community sizes. The parameter with value 0.5 is the mixing parameter; for each vertex roughly half of the edges will be within the planted cluster and half will be external. We believe that this setting means that recovering the planted clusters for the resulting graph is difficult.

For \(\gamma\) we will use 2.5, 3.0, and 3.5. For each, we will generate 1001 graphs using the seeds 0 through 1000. Later, we will also raise the mixing parameter to 0.6 to consider even harder problems where 60\% of the edges are external to the clusters.

4. Finding clusterings and measuring their quality

Given an LFR graph, we wish to find a division of the vertices into clusters. We use the Greedy Modularity algorithm [7] to do so. This algorithm is fairly simple: start with the clustering of all vertices in their own cluster and, at each step, if combining any two clusters improves the modularity, combine the two that give the greatest modularity. Ties can arise; our implementation relies on sorting the improvements and so should return the same answer on each run—we suspect that this performs roughly the same as randomly breaking ties.

We chose this algorithm for its simplicity. Our intention is not to measure the capability of the algorithm but rather the score on which it is climbing. We hope that using a simple algorithm will emphasize the differences in the quality of the score. We assume that more involved algorithms, for example the Louvain algorithm [3], will also perform better given a better score.

Along with the authors of [11], we believe that the best way to evaluate our found clusters is to look at whether individual pairs are correctly clustered together or apart. To be explicit, each pair of vertices has a true label, clustered together or not, from the planted clusters as well as a learned label from the clusters we produced via Greedy Modularity. The \(\binom{1000}{2}\) pairs of vertices are mostly not in the same cluster, so we have unbalanced class labels. Following the recommendation in [5] and elsewhere, we use the Matthews correlation coefficient [13] to turn the resulting 2 \times 2 confusion matrix into a single number. We rely on the implementation of the Matthews correlation coefficient in Scikit-learn [16].
5. Clustering using modularity

We begin by identifying the right resolution to use for our LFR graphs, Figure 2. We have plotted the median and quartiles of the Matthews correlation coefficient between the found clustering and the ground truth clustering; because we used 1001 graphs, these represent the results from particular graphs. Graphs with larger $\gamma$ prove to be harder to cluster; we contend that this is because they contain a larger proportion of low degree vertices. We use the greatest median to identify the best choice of resolution, which is 0.39 for $\gamma = 2.5$, 0.38 for $\gamma = 3.0$, and 0.37 for $\gamma = 3.5$.

We looked further at the three graphs that represent the median and quartile scores for $r = 0.39$ with $\gamma = 2.5$. In the top row of Figure 3 on the next page we plot the Matthews correlation coefficient between the true clusters and the recovered clusters when we restrict to pairs of vertices with certain degrees. For the leftmost figure, the bottom row represents vertices of degrees 14 through 18, of which there are 85. The lower left square represents all pairs of vertices with those degrees. The final box as we slide to the right in that triangle represents pairs where one vertex has degree 14 through 18 and the other degree 48 through 61; there are only 61 such vertices, so the block is narrower. Degrees are divided from smallest to largest with a break when the size of the current block would exceed 100 if we included the next degree. The next row up represents pairs involving vertices with degrees 19 or 20.

Looking at these results, a reasonable interpretation is that when both of the vertices have a relatively high degree, we can do pretty well at determining whether the two vertices should be clustered together or not. However, when at least one of the vertices has low degree, we do a poor job. Perhaps this is an inherent
Figure 3. Comparing Matthews correlation coefficient on different degree ranges. From left to right we have results for three LFR graphs with $\gamma = 2.5$; the top row represents the clustering found using modularity (\(Q_r\) of (2) with \(r = 0.39\)) and the bottom row the clustering found using flat modularity (\(Q^\text{♭}_R\) of (3) with \(R = 98\)). Within a figure, each block represents the Matthews correlation coefficient of the found clustering to the true clustering when we restrict to pairs of vertices with given degrees. The lowest row represents pairs involving vertices with the smallest degrees and the rightmost column represents pairs involving vertices with the largest degrees. A larger MCC is better.

problem. With higher-degree vertices, we see more of their neighbors and so have more information about who they should cluster with. With lower-degree vertices, we have less information and so clustering them is harder.

However, it’s also possible that the form of modularity is detrimental to our ability to cluster the lower-degree vertices. Making a change to modularity might be a way to improve the performance on lower-degree vertices. We attempt this next.

6. Flat modularity

For modularity, the penalty term arises from averaging the contribution over all graphs (which may have multiple edges or loops) on this set of vertices for which the vertices have their observed degrees. One can also interpret this as the expected value if we randomly reconnect the half-edges emerging from each vertex.
We proceed by averaging over a larger class of graphs, all graphs on the same vertices with the same number of edges. This changes the expected value, resulting in the formula

$$\frac{1}{2L} \sum_v \sum_w C_{vw} \left( A_{vw} - \frac{\hat{k}\hat{k}}{2L} \right)$$

where $\hat{k}$ is the average degree of the vertices of the graph. When we compare with the usual modularity [1], we see that the penalty term is flat (or uniform) over all pairs of vertices and so we call this flat modularity. Our hope is that by not having the penalty focus on pairs of high-degree vertices, we can achieve better performance in clustering the low-degree vertices; we expect the additional information about high-degree vertices to sustain our ability to cluster them well.

It’s natural to think that we would want to add a resolution to flat modularity as well. This becomes

$$\frac{1}{2L} \sum_v \sum_w C_{vw} \left( r \cdot A_{vw} - \frac{\hat{k}\hat{k}}{2L} \right).$$

In the statistical optimization literature or the machine learning literature, it is common to subtract a regularizer which is multiplied by some weight, usually denoted $\lambda$, that also needs to be learned. In order to get the weight onto the penalty side, we scale the above formula by $1/r$, arriving at

$$\frac{1}{2L} \sum_v \sum_w C_{vw} \left( A_{vw} - \frac{\hat{k}\hat{k}/r}{2L} \right).$$

In the formula above, the numerator of the penalty is some constant written in a complicated way. We replace it with a separate constant, arriving at our final formula for flat modularity,

$$Q^\flat = \frac{1}{2L} \sum_v \sum_w C_{vw} \left( A_{vw} - \frac{R}{2L} \right)$$

We’ve chosen to retain the $2L$ in the denominator of the penalty in order that the formula more closely resemble the formula for standard modularity. We assume this aesthetic decision will have little effect on performance but that is an open question.

As the degrees of the vertices are no longer relevant to the score, a clustering algorithm that relies on modularity no longer needs to track these degrees. This may simplify some implementations, though we note that each vertex does need to know what vertices it is adjacent to.

For the resolution, $r$, we considered values to two decimal places between 0 and 1. When we found that the optimal value of $R$ would be around 100, we decided to restrict $R$ to even integers between 0 and 200. The median and quartiles of the Matthews correlation coefficient when we apply the Greedy Modularity algorithm with flat modularity as the score are depicted in Figure 4 on the facing page.

Among other features, it is still the case that increasing $\gamma$ hurts our ability to recover the true clustering. The scores are also less smooth as a function of the penalty multiplier. This might be because there are more ties now; for modularity, the varying penalty is likely to drive down the number of ties. We collect the best scores we found in Table 1 on the next page. Using flat modularity has improved
the fidelity to the planted clustering and the relative decrease in performance with rising $\gamma$ is less when we use flat modularity.

The second row of Figure 3 on page 5 depicts the results of clustering using flat modularity on the same three graphs whose results in clustering using modularity are depicted in the first row. Switching to flat modularity does not hurt the performance in clustering high-degree vertices but does improve clustering of low-degree vertices. This is particularly evident in the lower right of the triangles which have become much darker. Therefore, we have done a better job matching low-degree vertices with high-degree vertices. The lower lefts of the triangles indicate there is still room for improvement in properly matching low-degree vertices amongst themselves, though we note that this is likely to be difficult in general.
Table 2. Median and quartiles of the Matthews correlation coefficient over pairs where one vertex has degree at most 20 and one degree at least 40 split between climbing using modularity with the best resolution we found and using flat modularity with the best penalty multiplier we found; a larger MCC is better.

| $\gamma$ | $r$ | 1/4-ile | Median | 3/4-ile | $R$ | 1/4-ile | Median | 3/4-ile |
|---------|-----|---------|--------|---------|-----|---------|--------|---------|
| 2.5     | 0.39| 0.1705  | 0.2115 | 0.2538  | 98  | 0.2243  | 0.2661 | 0.3142  |
| 3.0     | 0.38| 0.1774  | 0.2154 | 0.2607  | 98  | 0.2283  | 0.2702 | 0.3189  |
| 3.5     | 0.37| 0.1798  | 0.2224 | 0.2647  | 98  | 0.2266  | 0.2701 | 0.3216  |

These observations generally hold for all of the graphs. We computed the Matthews correlation coefficient between the found clustering and the true clustering restricted to pairs of vertices where one has degree at most 20 and one degree at least 40. This corresponds to the lower right of our triangles. The medians and quartiles over the 1001 graphs are found in Table 2; the $r$ and $R$ values are the ones from Table 1; we did not attempt to find the best $r$ and $R$ for this set of vertices. This supports the claim that using flat modularity leads to improved clustering of low-degree vertices. Note that the observed values for these pairs are more similar for the different values of $\gamma$ than what we observed in Table 1. We posit that there is relatively consistent performance among pairs of high-degree vertices, among pairs of low-degree vertices, and among pairs where one is low-degree and the other high-degree. Therefore, the change in performance with different $\gamma$’s is due to the change in the numbers of each type of pair.

For each of the 1001 graphs with $\gamma = 2.5$, we have plotted the Matthews correlation coefficient of the found clustering using standard modularity with resolution $r = 0.39$ against the Matthews correlation coefficient from using flat modularity with multiplier $R = 98$ in Figure 5 on the facing page. We do not see, for example, that the improvement only comes from graphs where the original climb did particularly poorly; rather there is general improvement. We have not done any analysis to identify features of the graphs that might correlate with either score or the difference in the scores.

We repeated these experiments with the mixing parameter set to 0.6 instead of the 0.5 of the main text. We record the results that correspond to Tables 1 and 2 in Table 3 on page 10. As in the 0.5 case, we chose $r$ and $R$ to maximize the median Matthews correlation coefficient between the planted clusters and the found clusters over all of the vertices and, for those values of $r$ and $R$, we report out statistics for the Matthews correlation coefficient between the planted clustering and the found clustering restricted to pairs of vertices where one vertex has degree at most 20 and one degree at least 40. In this harder case, there is again a large difference in favor of flat modularity in both the overall scores and restricted to pairs that involve one low-degree vertex and one high-degree vertex.
Conclusions

Modularity continues to be a factor in finding clusters in graphs. If we interpret modularity as involving a bonus and a penalty, then the penalty is higher for higher-degree vertices. When we use a simple clustering algorithm that attempts to maximize modularity, it fares far better on the high-degree vertices than on the low-degree vertices.

We therefore ask whether it is better to have the penalty be independent of the degree of the vertex. We found that the same simple algorithm, now using flat modularity, finds clusterings that better match the ground truth, in particular improving the clustering of lower-degree vertices. Meanwhile, our implementation became simpler because we no longer needed to track the degrees of the vertices.

We have more information about the vertices with higher degrees and so it is not surprising that we can cluster them more effectively. Having our penalty focus on this high information region proves less helpful than flattening the penalty. Perhaps one could even go further and try to apply the penalty disproportionately to low-degree vertices; we have not tested this idea.

While our tests were confined to graphs in which the vertex degrees satisfy a power law, we expect the results to generalize to other heavy-tailed degree distributions. Since such graphs occur frequently, and finding communities in graphs
Table 3. Median and quartiles of the Matthews correlation coefficient for either all pairs of vertices or only pairs where one vertex has degree at most 20 and one degree at least 40 split between climbing using modularity with the best resolution we found and using flat modularity with the best penalty multiplier we found over 1001 graphs where the mixing parameter was 0.6; a larger MCC is better. The chosen values of $r$ and $R$ maximize the median Matthews correlation over all pairs of vertices.

|                | Modularity          | Flat modularity     |
|----------------|---------------------|---------------------|
|                | $r$ | 1/4-ile | Median | 3/4-ile | $R$ | 1/4-ile | Median | 3/4-ile |
| All pairs      |     |         |        |         |     |         |        |         |
| 2.5            | 0.39| 0.0792  | 0.1072 | 0.1322  | 106 | 0.1535  | 0.1880 | 0.2186  |
| 3.0            | 0.39| 0.0723  | 0.0949 | 0.1177  | 106 | 0.1386  | 0.1700 | 0.2032  |
| 3.5            | 0.44| 0.0630  | 0.0861 | 0.1060  | 106 | 0.1225  | 0.1529 | 0.1826  |
| Pairs with a low-degree vertex and a high-degree vertex only | | | |
| 2.5            | 0.39| 0.0188  | 0.0271 | 0.0383  | 106 | 0.0328  | 0.0468 | 0.0649  |
| 3.0            | 0.39| 0.0231  | 0.0334 | 0.0465  | 106 | 0.0379  | 0.0535 | 0.0728  |
| 3.5            | 0.44| 0.0263  | 0.0363 | 0.0484  | 106 | 0.0422  | 0.0588 | 0.0804  |

continues to be an important problem, we believe that the simple change from modularity to flat modularity can improve a broad range of clustering results with minimal change to implementations.

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