Notes on Louvain Modularity

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1 Undirected Modularity

This section is motivated by the application of the Louvain modularity clustering algorithm to an undirected graph, as (incompletely) described by [1].

Let $D_{ij} \geq 0$ represent the weight of a directed edge $i \rightarrow j$ (if one exists) from vertex $i \in \mathcal{V}$ to vertex $j \in \mathcal{V}$. Then the equivalent undirected edge has weight $A_{ij} = D_{ij} + D_{ji} - \delta_{ij} D_{ii}$, such that $A_{ij} = A_{ji}$. The total weight of all edges for vertex i (its so-called *vertex weight*) is then given by

$$A_{i\cdot} \;=\; \sum_{j\in\mathcal{V}} A_{ij} \;=\; \sum_{j\in\mathcal{V}} A_{ji} \;=\; A_{\cdot i}\,. \tag{1.1}$$

The sum of all vertex weights is then given by

$$A_{\cdot\cdot} \;=\; \sum_{i\in\mathcal{V}} A_{i\cdot} \;=\; \sum_{i\in\mathcal{V}} \sum_{j\in\mathcal{V}} A_{ij}\,. \tag{1.2}$$

Note that this counts self edges (i.e. $i - i$) once and all other edges (i.e. $i - j$, $i \neq j$) twice. The Louvain modularity algorithm [1] in fact assumes that there are no self edges, but we shall include them here for completeness.

The modularity score of a clustered, undirected graph is then given by

$$Q \;=\; \sum_{i\in\mathcal{V}} \sum_{j\in\mathcal{V}} \left[\frac{A_{ij}}{A_{\cdot\cdot}} - \frac{A_{i\cdot}A_{\cdot j}}{A_{\cdot\cdot}^2}\right] \delta(c_i, c_j)\,, \tag{1.3}$$

where c_i is the index of the cluster containing vertex i. Note that $\delta(c_i, c_j) = 1$ if and only if $c_i = c_j = g$ for some cluster index g. Then Q can be partitioned by cluster as

$$Q \;=\; \sum_{g=1}^{G} \sum_{i\in\mathcal{V}_g} \sum_{j\in\mathcal{V}_g} \left[\frac{A_{ij}}{A_{\cdot\cdot}} - \frac{A_{i\cdot}A_{\cdot j}}{A_{\cdot\cdot}^2}\right] \;\doteq\; \sum_{g=1}^{G} Q_g\,, \tag{1.4}$$

where the g-th cluster contains vertices $\mathcal{V}_g = \{i \in \mathcal{V} \mid c_i = g\}$, and therefore $\mathcal{V} = \bigcup_{g=1}^{G} \mathcal{V}_g$.

We now observe that the sum of edge weights of vertex i for all edges to and from cluster g is given by

$$A_{i,g} \;=\; \sum_{j\in\mathcal{V}_g} A_{ij}\,, \tag{1.5}$$

and hence the *internal* cluster weight, namely the total weight of all edges internal to cluster g, is given by

$$\Sigma_g^{\mathtt{int}} \;=\; \sum_{i\in\mathcal{V}_g} \sum_{j\in\mathcal{V}_g} A_{ij} \;=\; \sum_{i\in\mathcal{V}_g} A_{i,g}\,. \tag{1.6}$$

Note that this value, like $A_{\cdot\cdot}$, also counts self edges $(i - i)$ once and all other edges $(i - j)$ twice. Conversely, the *external* cluster weight, namely the total weight of all edges from vertices in cluster g to and from vertices in other clusters, is given by

$$\Sigma_g^{\mathtt{ext}} \;=\; \sum_{i\in\mathcal{V}_g} \sum_{j\in\bar{\mathcal{V}}_g} A_{ij} \;=\; \sum_{j\in\bar{\mathcal{V}}_g} A_{j,g}\,, \tag{1.7}$$

where $\bar{\mathcal{V}}_g = \mathcal{V}\backslash\mathcal{V}_g$ (or $\mathcal{V} - \mathcal{V}_g$). Note that these external edge weights are only counted once per cluster, but the edge $i - j$ is counted separately for both the cluster containing vertex i and the other cluster containing vertex j.

The total weight of cluster g is then given by

$$\begin{aligned}\Sigma_g^{\mathtt{tot}} &= \Sigma_g^{\mathtt{int}} + \Sigma_g^{\mathtt{ext}} \\ &= \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g} A_{ij} + \sum_{i\in\mathcal{V}_g}\sum_{j\in\bar{\mathcal{V}}_g} A_{ij} \\ &= \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}} A_{ij} \;=\; \sum_{i\in\mathcal{V}_g} A_{i\cdot}\,. \end{aligned} \tag{1.8}$$

We now observe that

$$\begin{aligned}\sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g} A_{i\cdot}A_{\cdot j} &= \sum_{i\in\mathcal{V}_g} A_{i\cdot}\sum_{j\in\mathcal{V}_g} A_{\cdot j} \\ &= \left(\sum_{i\in\mathcal{V}_g} A_{i\cdot}\right)\left(\sum_{j\in\mathcal{V}_g} A_{j\cdot}\right) \\ &= \left(\sum_{i\in\mathcal{V}_g} A_{i\cdot}\right)^2 \;=\; \left(\Sigma_g^{\mathtt{tot}}\right)^2\,. \end{aligned} \tag{1.9}$$

Hence, from equation (1.4), we see that the modularity score of the g-th cluster simplifies to become

$$Q_g \;=\; \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g}\left[\frac{A_{ij}}{A_{\cdot\cdot}} - \frac{A_{i\cdot}A_{\cdot j}}{A_{\cdot\cdot}^2}\right] \;=\; \frac{\Sigma_g^{\mathtt{int}}}{A_{\cdot\cdot}} - \left(\frac{\Sigma_g^{\mathtt{tot}}}{A_{\cdot\cdot}}\right)^2\,, \tag{1.10}$$

from equations (1.6) and (1.9).

This cluster modularity score Q_g now gives us a handle on how to compute changes in score due to changes in the graph clustering, with the aim of choosing a clustering that maximises the total modularity score Q. Suppose we merge a singleton cluster containing only vertex k with another cluster g to form a new cluster $g \oplus k$ (technically, the new cluster is $\mathcal{V}_{g\oplus k} = \mathcal{V}_g \bigcup\{k\}$). Then, from equation (1.6), the new internal cluster weight is given by

$$\begin{aligned}\Sigma_{g\oplus k}^{\mathtt{int}} &= \sum_{i\in\mathcal{V}_g\bigcup\{k\}}\;\sum_{j\in\mathcal{V}_g\bigcup\{k\}} A_{ij} \\ &= \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g} A_{ij} + \sum_{i\in\mathcal{V}_g} A_{ik} + \sum_{j\in\mathcal{V}_g} A_{kj} + A_{kk} \\ &= \Sigma_g^{\mathtt{int}} + 2A_{k,g} + A_{kk}\,. \end{aligned} \tag{1.11}$$

Similarly, the new total cluster weight is given by

$$\Sigma_{g\oplus k}^{\mathtt{tot}} \;=\; \sum_{i\in\mathcal{V}_g\bigcup\{k\}} A_{i\cdot} \;=\; \sum_{i\in\mathcal{V}_g} A_{i\cdot} + A_{k\cdot} \;=\; \Sigma_g^{\mathtt{tot}} + A_{k\cdot}\,, \tag{1.12}$$

from equation (1.8). Consequently, the modularity score of the new cluster is given by

$$\begin{aligned}Q_{g\oplus k} &= \frac{\Sigma_{g\oplus k}^{\mathtt{int}}}{A_{\cdot\cdot}} - \left(\frac{\Sigma_{g\oplus k}^{\mathtt{tot}}}{A_{\cdot\cdot}}\right)^2 \\ &= \frac{\Sigma_g^{\mathtt{int}} + 2A_{k,g} + A_{kk}}{A_{\cdot\cdot}} - \left(\frac{\Sigma_g^{\mathtt{tot}} + A_{k\cdot}}{A_{\cdot\cdot}}\right)^2\,, \end{aligned} \tag{1.13}$$

from equations (1.10)–(1.12). By extension, a singleton cluster containing only vertex k is notionally formed by merging the vertex with an empty cluster having zero cluster weights, and so the modularity score of the singelton cluster is just

$$Q_k \;=\; \frac{A_{kk}}{A_{\cdot\cdot}} - \left(\frac{A_{k\cdot}}{A_{\cdot\cdot}}\right)^2\,. \tag{1.14}$$

Note that the Louvain modularity algorithm [1] starts by placing every vertex $k \in \mathcal{V}$ into its own singleton cluster, and so initially there are $G = |\mathcal{V}|$ such clusters. Also note that, as mentioned above, the Louvain algorithm [1] implicitly assumes that $A_{kk} = 0$.

We can now compute the total change in modularity caused by adding singleton vertex k to cluster g, namely

$$\begin{aligned}
\Delta Q_{(g,k)\to g\oplus k} &= Q_{g\oplus k} - Q_g - Q_k \\
&= \left[\frac{\Sigma_g^{\mathtt{int}} + 2A_{k,g} + A_{kk}}{A_{\cdot\cdot}} - \left(\frac{\Sigma_g^{\mathtt{tot}} + A_{k\cdot}}{A_{\cdot\cdot}}\right)^2\right] - \left[\frac{\Sigma_g^{\mathtt{int}}}{A_{\cdot\cdot}} - \left(\frac{\Sigma_g^{\mathtt{tot}}}{A_{\cdot\cdot}}\right)^2\right] - \left[\frac{A_{kk}}{A_{\cdot\cdot}} - \left(\frac{A_{k\cdot}}{A_{\cdot\cdot}}\right)^2\right] \\
&= \frac{\Sigma_g^{\mathtt{int}} + 2A_{k,g} + A_{kk}}{A_{\cdot\cdot}} - \frac{(\Sigma_g^{\mathtt{tot}})^2 + 2\Sigma_g^{\mathtt{tot}}A_{k\cdot} + A_{k\cdot}^2}{A_{\cdot\cdot}^2} - \frac{\Sigma_g^{\mathtt{int}} + A_{kk}}{A_{\cdot\cdot}} + \frac{(\Sigma_g^{\mathtt{tot}})^2 + A_{k\cdot}^2}{A_{\cdot\cdot}^2} \\
&= \frac{2A_{k,g}}{A_{\cdot\cdot}} - \frac{2\Sigma_g^{\mathtt{tot}}A_{k\cdot}}{A_{\cdot\cdot}^2}\,, \qquad (1.15)
\end{aligned}$$

from equations (1.10) and (1.13)–(1.14). Conceptually, this is just the score change upon destroying clusters k and g and then creating a new cluster $g \oplus k$.

In the converse situation, we instead want to remove vertex k from the cluster $g \oplus k$ and restore k to its singleton cluster. Since the action of adding vertex k to group g (above) is reversible, then removing the vertex must result in a change of modularity score opposite to the change in score caused by adding the vertex. This is just the score change involved in destroying cluster $g \oplus k$ and creating clusters g and k. Hence, we obtain

$$\Delta Q_{g\oplus k\to(g,k)} = Q_g + Q_k - Q_{g\oplus k} = -\frac{2A_{k,g}}{A_{\cdot\cdot}} + \frac{2\Sigma_g^{\mathtt{tot}}A_{k\cdot}}{A_{\cdot\cdot}^2}\,, \qquad (1.16)$$

where now $A_{k,g}$ is computed from $A_{k,g\oplus k}$ via

$$\begin{aligned}
A_{k,g\oplus k} &= \sum_{j\in\mathcal{V}_g \bigcup\{k\}} A_{kj} = \sum_{j\in\mathcal{V}_g} A_{kj} + A_{kk} = A_{k,g} + A_{kk} \\
\Rightarrow A_{k,g} &= A_{k,g\oplus k} - A_{kk}\,, \qquad (1.17)
\end{aligned}$$

and $\Sigma_g^{\mathtt{tot}}$ is computed from $\Sigma_{g\oplus k}^{\mathtt{tot}}$ as

$$\Sigma_g^{\mathtt{tot}} = \Sigma_{g\oplus k}^{\mathtt{tot}} - A_{k\cdot}\,, \qquad (1.18)$$

from equation (1.12). In terms of the existing cluster $g \oplus k$, the score change is thus

$$\Delta Q_{g\oplus k\to(g,k)} = -\frac{2(A_{k,g\oplus k} - A_{kk})}{A_{\cdot\cdot}} + \frac{2(\Sigma_{g\oplus k}^{\mathtt{tot}} - A_{k\cdot})A_{k\cdot}}{A_{\cdot\cdot}^2}\,. \qquad (1.19)$$

Hence, the combined action of removing vertex k from cluster $g \oplus k$ (to form cluster g) and adding it to cluster g' (to form cluster $g' \oplus k$) gives rise to the total change of score

$$\Delta Q_{(g\oplus k,g')\to(g,g'\oplus k)} = \Delta Q_{g\oplus k\to(g,k)} + \Delta Q_{(g',k)\to g'\oplus k}\,, \qquad (1.20)$$

utilising equations (1.15) and (1.19).

2 Directed Modularity

This section is motivated by the application of the Louvain modularity clustering algorithm to a directed graph, as described by [2]. In distinction from the case of Section 1, we now take $A_{ij} = D_j \geq 0$ to be the directed edge weight from vertex i to vertex j (if such an edge exists), such that $A_{ij} \neq A_{ji}$ in general; this breaks a number of assumptions used in Section1. For example, equation (1.1) now becomes

$$s_i^{\mathtt{out}} = A_{i\cdot} = \sum_{j\in\mathcal{V}} A_{ij}\,, \qquad s_j^{\mathtt{in}} = \sum_{i\in\mathcal{V}} A_{ij} = A_{\cdot j}\,, \qquad (2.1)$$

mixing in some of the notation from [2]. Similarly, if we consider the g-th cluster, then the external cluster weight from equation (1.7) is now replaced by

$$\Sigma_g^{\mathtt{out}} = \sum_{i\in\mathcal{V}_g}\sum_{j\in\bar{\mathcal{V}}_g} A_{ij}\,, \qquad \Sigma_g^{\mathtt{in}} = \sum_{i\in\bar{\mathcal{V}}_g}\sum_{j\in\mathcal{V}_g} A_{ij}\,, \qquad (2.2)$$

such that

$$S_g^{\mathtt{out}} \;=\; \sum_{i\in\mathcal{V}_g} s_i^{\mathtt{out}} \;=\; \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}} A_{ij} \;=\; \Sigma_g^{\mathtt{int}} + \Sigma_g^{\mathtt{out}}\,, \tag{2.3}$$

and

$$S_g^{\mathtt{in}} \;=\; \sum_{j\in\mathcal{V}_g} s_j^{\mathtt{in}} \;=\; \sum_{i\in\mathcal{V}}\sum_{j\in\mathcal{V}_g} A_{ij} \;=\; \Sigma_g^{\mathtt{int}} + \Sigma_g^{\mathtt{out}}\,, \tag{2.4}$$

using equation (1.6). It follows that the modularity score Q_g of the g-th cluster becomes

$$Q_g \;=\; \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g}\left[\frac{A_{ij}}{A_{\cdot\cdot}} - \frac{A_{i\cdot}A_{\cdot j}}{A_{\cdot\cdot}^2}\right] \;=\; \frac{\Sigma_g^{\mathtt{int}}}{A_{\cdot\cdot}} - \frac{S_g^{\mathtt{out}}S_g^{\mathtt{in}}}{A_{\cdot\cdot}^2}\,, \tag{2.5}$$

instead of equation (1.10).

We now consider the effect of merging the g-th cluster with the singleton cluster containing only vertex k, resulting in a new cluster $g\oplus k$. The internal weight $\Sigma_{g\oplus k}^{\mathtt{int}}$ of this new cluster is now no longer given by equation (1.11), but instead by

$$\begin{aligned}
\Sigma_{g\oplus k}^{\mathtt{int}} &= \sum_{i\in\mathcal{V}_g\bigcup\{k\}}\;\sum_{j\in\mathcal{V}_g\bigcup\{k\}} A_{ij}\\
&= \sum_{i\in\mathcal{V}_g}\sum_{j\in\mathcal{V}_g} A_{ij} + \sum_{i\in\mathcal{V}_g} A_{ik} + \sum_{j\in\mathcal{V}_g} A_{kj} + A_{kk}\\
&= \Sigma_g^{\mathtt{int}} + W(g,k) + W(k,g) + A_{kk}\,.
\end{aligned} \tag{2.6}$$

More generally, $W(g,k)$ is the edge weight from all vertices in the g-th cluster to vertex k, excluding any self edge $k\to k$ if k happens to be a member of the g-th cluster. Thus

$$W(g,k) \;=\; \sum_{\substack{i\in\mathcal{V}_g\\ i\neq k}} A_{ik}\,, \tag{2.7}$$

and conversely

$$W(k,g) \;=\; \sum_{\substack{j\in\mathcal{V}_g\\ j\neq k}} A_{kj}\,, \tag{2.8}$$

which is the edge weight from vertex k to all vertices (except k) in the g-th cluster.

Similarly, the cluster merge $g\oplus k$ results in new out and in edge weights given by

$$S_{g\oplus k}^{\mathtt{out}} \;=\; \sum_{i\in\mathcal{V}_g\bigcup\{k\}} A_{i\cdot} \;=\; \sum_{i\in\mathcal{V}_g} A_{i\cdot} + A_{k\cdot} \;=\; S_g^{\mathtt{out}} + s_k^{\mathtt{out}}\,, \tag{2.9}$$

$$S_{g\oplus k}^{\mathtt{in}} \;=\; \sum_{j\in\mathcal{V}_g\bigcup\{k\}} A_{\cdot j} \;=\; \sum_{j\in\mathcal{V}_g} A_{\cdot j} + A_{\cdot k} \;=\; S_g^{\mathtt{out}} + s_k^{\mathtt{in}}\,, \tag{2.10}$$

respectively; these equations supercede equation (1.12). Consequently, the modularity score of the new cluster is now given by

$$\begin{aligned}
Q_{g\oplus k} &= \frac{\Sigma_{g\oplus k}^{\mathtt{int}}}{A_{\cdot\cdot}} - \frac{S_{g\oplus k}^{\mathtt{out}}S_{g\oplus k}^{\mathtt{in}}}{A_{\cdot\cdot}^2}\\
&= \frac{\Sigma_g^{\mathtt{int}} + W(g,k) + W(k,g) + A_{kk}}{A_{\cdot\cdot}} - \frac{\left(S_g^{\mathtt{out}} + A_{k\cdot}\right)\left(S_g^{\mathtt{in}} + A_{\cdot k}\right)}{A_{\cdot\cdot}^2}\,,
\end{aligned} \tag{2.11}$$

instead of by equation (1.13). Similarly, the modularity score of the singleton cluster k is now just

$$Q_k \;=\; \frac{A_{kk}}{A_{\cdot\cdot}} - \frac{A_{k\cdot}A_{\cdot k}}{A_{\cdot\cdot}^2}\,, \tag{2.12}$$

replacing equation (1.14). Finally, the change in score due to merging clusters g and k is

$$\begin{aligned}
\Delta Q_{(g,k)\to g\oplus k} &= Q_{g\oplus k} - Q_g - Q_k \\
&= \left[\frac{\Sigma_g^{\mathtt{int}} + W(g,k) + W(k,g) + A_{kk}}{A_{\cdot\cdot}} - \frac{\left(S_g^{\mathtt{out}} + A_{k\cdot}\right)\left(S_g^{\mathtt{in}} + A_{\cdot k}\right)}{A_{\cdot\cdot}^2}\right] \\
&\quad - \left[\frac{\Sigma_g^{\mathtt{int}}}{A_{\cdot\cdot}} - \frac{S_g^{\mathtt{out}} S_g^{\mathtt{in}}}{A_{\cdot\cdot}^2}\right] - \left[\frac{A_{kk}}{A_{\cdot\cdot}} - \frac{A_{k\cdot} A_{\cdot k}}{A_{\cdot\cdot}^2}\right] \\
&= \frac{W(g,k) + W(k,g)}{A_{\cdot\cdot}} - \frac{S_g^{\mathtt{out}} A_{\cdot k} + S_g^{\mathtt{in}} A_{k\cdot}}{A_{\cdot\cdot}^2}\,,
\end{aligned} \tag{2.13}$$

which replaces equation (1.15).

We can now compute the change in modularity score involved with removing vertex k from some cluster $g \oplus k$, resulting in cluster g. As in Section 1, this is just the negative of the score change from merging vertex k with cluster g, namely

$$\begin{aligned}
\Delta Q_{g\oplus k\to(g,k)} &= -\frac{W(g,k) + W(k,g)}{A_{\cdot\cdot}} + \frac{S_g^{\mathtt{out}} A_{\cdot k} + S_g^{\mathtt{in}} A_{k\cdot}}{A_{\cdot\cdot}^2} \\
&= -\frac{W(g\oplus k,k) + W(k,g\oplus k)}{A_{\cdot\cdot}} + \frac{(S_{g\oplus k}^{\mathtt{out}} - A_{k\cdot})A_{\cdot k} + (S_{g\oplus k}^{\mathtt{in}} - A_{\cdot k})A_{k\cdot}}{A_{\cdot\cdot}^2}\,,
\end{aligned} \tag{2.14}$$

from equations (2.7)–(2.8) and (2.9)–(2.10). This replaces equation (1.19). The total change in modularity score involved in moving vertex k from cluster $g \oplus k$ to some other cluster g' is therefore

$$\begin{aligned}
\Delta Q_{(g\oplus k,g')\to(g,g'\oplus k)} &= \Delta Q_{g\oplus k\to(g,k)} + \Delta Q_{(g',k)\to g'\oplus k} \\
&= \frac{W(g',k) + W(k,g') - W(g\oplus k,k) - W(k,g\oplus k)}{A_{\cdot\cdot}} \\
&\quad - \frac{(S_{g'}^{\mathtt{out}} - S_{g\oplus k}^{\mathtt{out}} + A_{k\cdot})A_{\cdot k} + (S_{g'}^{\mathtt{in}} - S_{g\oplus k}^{\mathtt{in}} + A_{\cdot k})A_{k\cdot}}{A_{\cdot\cdot}^2}\,.
\end{aligned} \tag{2.15}$$

This is essentially equation (3.26) of [2] (with ΔQ scaled by $A_{\cdot\cdot}$), except that their use of m (the total number of edges) should be replaced with $m_w = A_{\cdot\cdot}$ (the total weight of all edges).

References

[1] Vincent D Blondel, Jean-Loup Guillaume, Renaud Lambiotte, Etienne Lefebvre, *Fast unfolding of communities in large networks*, Journal of Statistical Mechanics: Theory and Experiment 2008 (10), P10008; ArXiv: https://arxiv.org/abs/0803.0476.

[2] Arnaud Browet, *Algorithms for community and role detection in networks*, Doctoral thesis, Louvain-la-Neuve, September 30, 2014; https://perso.uclouvain.be/arnaud.browet/files/thesis/thesis.pdf.