Notes on Louvain Modularity

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1 Modularity

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 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 $\bar{\mathcal{V}}_g = \mathcal{V} - \mathcal{V}_g$. 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

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

We now observe that

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

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

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

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 $g \oplus k$. Then, from equation (1.6), the new internal cluster weight is given by

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

Similarly, the new total cluster weight is given by

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

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

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

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

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

Note that the Louvain modularity algorithm 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 published Louvain algorithm 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). 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

$$\Delta Q_{(g\oplus k,g')\to(g,g'\oplus k)} = \Delta Q_{g\oplus k\to(g,k)} + \Delta Q_{(g',k)\to g'\oplus k}\,, \qquad (1.19)$$

utilising equations (1.15)–(1.16).