

On Modularity Clustering

Presented by:
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Modularity

- A quality index for clustering a graph $G=(V,E)$

$$q(C) := \sum_{C \in \mathcal{C}} \left[\frac{|E(C)|}{m} - \left(\frac{|E(C)| + \sum_{C' \in \mathcal{C}} |E(C, C')|}{2m} \right)^2 \right]$$

This is equivalent to:

$$q(C) := \sum_{C \in \mathcal{C}} \left[\frac{|E(C)|}{m} - \left(\frac{\sum_{v \in C} \deg(v)}{2m} \right)^2 \right]$$

Contribution of the Paper

- Integer Linear Program Formulation
- Fundamental Observations & Counterintuitive Behavior
- NP- Completeness of Maximizing Modularity Problem
- A Greedy Algorithm
- Optimality Results

Maximizing Modularity via Integer Linear programming

Given a graph $G=(V,E)$, $n=|V|$ nodes, n^2 decision variables $X_{uv} \in \{0,1\}$

$$\text{Max: } q(C) := \frac{1}{2m} \sum_{(u,v) \in V^2} \left[E_{uv} - \frac{\deg(u)\deg(v)}{2m} \right] X_{uv}$$

St:

$$\forall u: X_{uu} = 1$$

$$\forall u, v: X_{uv} = X_{vu}$$

$$\forall u, v, w: X_{uv} + X_{vw} - 2X_{uw} \leq 1$$

$$\forall u, v: X_{uv} \in \{0,1\}$$

Fundamental Observations

If G is an undirected and un-weighted graph and C is a clustering then:

$$-1/2 \leq q(c) \leq 1$$

- *When all the edges are inter-cluster $q(C) = -1/2$, eg: Bipartite graph $G=(X:Y,E)$ with cluster X and Y*
- *When all the clusters cliques with no inter-cluster edges $q(C) = 1$, when number of clusters are infinite*

Fundamental Observations(Contd)

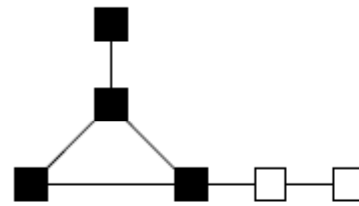
Clustering with maximum modularity has no cluster with single node having degree 1.

Fundamental Observations(Contd)

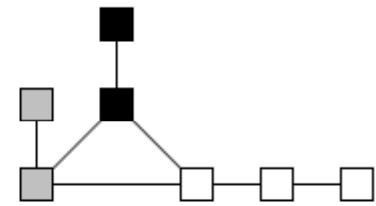
In clustering with maximum modularity each cluster consist of a connected sub-graph

Counterintuitive Behavior

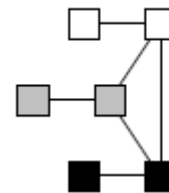
- Non-locality
- Sensitivity to Satellite
- Scaling Behavior



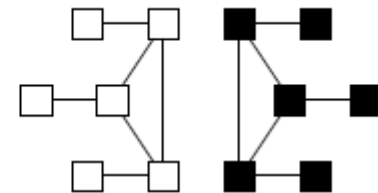
(a)



(b)



(c)



(d)

NP-Completeness

- *Problem 1 (Modularity):*

Given a graph G and a number K is there a clustering C of G , for which $q(C) \geq K$

- *Problem 2 (3-Partition):*

Given $3k$ positive integers numbers a_1, a_2, \dots, a_{3k} such that the sum $\sum_{i=1}^{3k} a_i = kb$ and $b/4 < a_i < b/2$ for an integer b and for all $i=1, 2, \dots, 3k$ is there a partition of these numbers into k sets, such that the numbers in each set sums upto b ?

NP-Completeness (contd)

- An instance $A = \{a_1, a_2, \dots, a_{3k}\}$ of 3-Partition can be transformed into an instance $(G(A), K(A))$ of Modularity
- $G(A)$ has a clustering with modularity at least $K(A)$, if and only if a_1, a_2, \dots, a_{3k} can be partitioned into k sets of sum $b = \frac{1}{k} \sum_{i=1}^{3k} a_i$

NP-Completeness (contd)

- Construct a graph $G(A)$ with k cliques H_1, H_2, \dots, H_k of size $a = \sum_{i=1}^{3k} a_i$ each.
- For each element $a_i \in A$ introduce a single element node. And connect it to a_i nodes in each of the k cliques.
- Each member of clique is connected to exactly one element node.
- Each clique node has degree a , each element node $a_i \in A$ has a degree ka_i .
- The number of edges in $G(A)$ is $m = (k/2)a(a+1)$

NP-Completeness (contd)

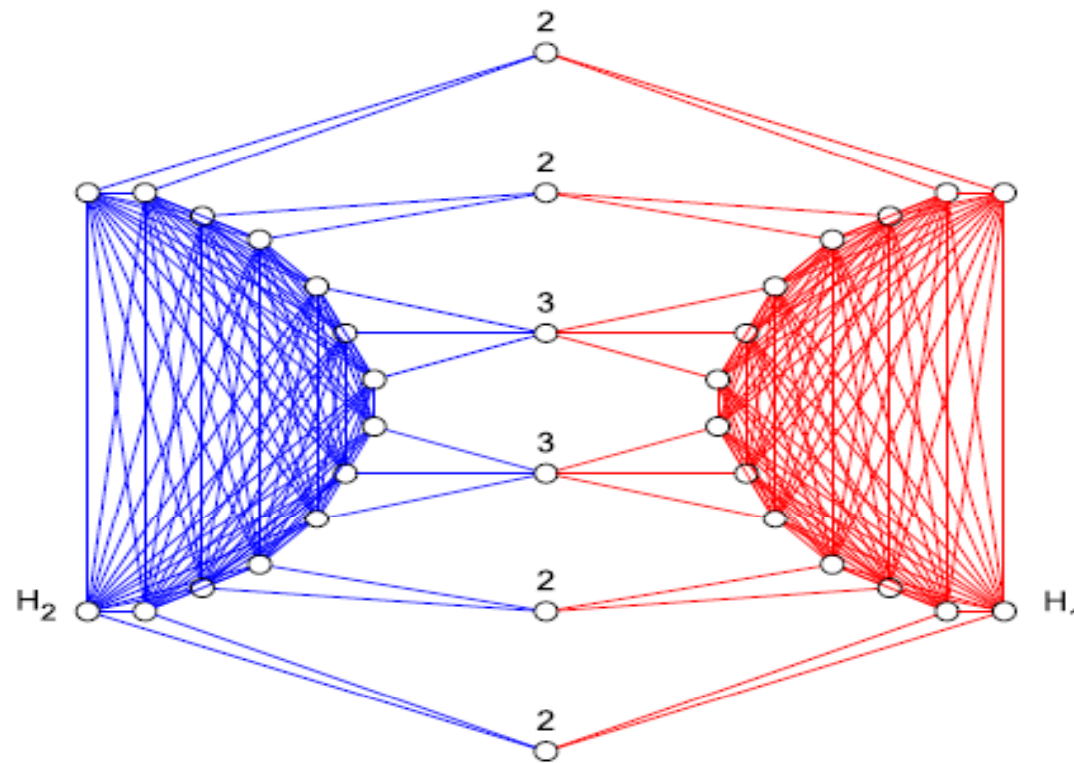


Fig. 2. An example graph $G(A)$ for the instance $A = \{2, 2, 2, 2, 3, 3\}$ of 3-PARTITION. Node labels indicate the corresponding numbers $a_i \in A$.

NP-Completeness (contd)

Lemma 4.1: In maximum modularity clustering of $G(A)$ none of the cliques H_1, H_2, \dots, H_k split.

- Clustering C splits a clique $H \in \{H_1, H_2, \dots, H_k\}$.
- $\{C_1, C_2, \dots, C_r\} \in C$ are clusters that contains the nodes of H .
- n_i is the number of nodes of H contained in cluster C_i
- $m_i = |E(C_i)|$ is the number of edges between nodes in C_i .
- f_i is the number of edges between the nodes of H and C_i .
- d_i is the sum of degree of all nodes in C_i .

NP-Completeness (contd)

The contribution of $\{C_1, C_2, \dots, C_r\} \in C$ to $q(C)$ is:

$$\frac{1}{m} \sum_{i=1}^r m_i - \frac{1}{4m^2} \sum_{i=1}^r d_i^2$$

Rearranging nodes in $\{C_1, C_2, \dots, C_r\} \in C$ into clusters $C', C_1', C_2', \dots, C_r'$ such that:

- C' contains the nodes of H
- And each C_i' contains the remaining nodes of C_i

NP-Completeness (contd)

- The contribution of $C', C_1', C_2', \dots, C_r'$ to $q(C')$ is given as

$$\frac{1}{m} \sum_{i=1}^r \left(m_i + \sum_{j=i+1}^r n_i n_j - f_i \right) - \frac{1}{4m^2} \left(a^4 + \sum_{i=1}^r (d_i - n_i a)^2 \right) .$$

Setting $\Delta := q(C') - q(C)$, we obtain

$$\begin{aligned} \Delta &= \frac{1}{m} \left(\sum_{i=1}^r \sum_{j=i+1}^r n_i n_j - f_i \right) \\ &\quad + \frac{1}{4m^2} \left(\left(\sum_{i=1}^r 2d_i n_i a - n_i^2 a^2 \right) - a^4 \right) \\ &= \frac{1}{4m^2} \left((4m \sum_{i=1}^r \sum_{j=i+1}^r n_i n_j - 4m \sum_{i=1}^r f_i \right. \\ &\quad \left. + \left(\sum_{i=1}^r n_i (2d_i a - n_i a^2) \right) - a^4 \right) . \end{aligned}$$

NP-Completeness (contd)

- Substituting $2\sum_{i=1}^r \sum_{j=i+1}^r n_i n_j = \sum_{i=1}^r \sum_{j \neq i} n_i n_j$ and $m = \frac{k}{2} a(a+1)$

$$\begin{aligned}\Delta &= \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i \right. \\ &\quad \left. + \sum_{i=1}^r n_i \left(2d_i - n_i a + k(a+1) \sum_{j \neq i} n_j \right) \right) \\ &\geq \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i \right. \\ &\quad \left. + \sum_{i=1}^r n_i \left(n_i a + 2k f_i + k(a+1) \sum_{j \neq i} n_j \right) \right)\end{aligned}$$

The fact that $n_i a + k f_i \leq d_i$ is used

NP-Completeness (contd)

- Combining n_i and one of the $\sum_{j \neq i} n_j$

$$\Delta \geq \frac{a}{4m^2} \left(-a^3 - 2k(a+1) \sum_{i=1}^r f_i \right) + \frac{a}{4m^2} \left(\sum_{i=1}^r n_i \left(a \sum_{j=1}^r n_j + 2kf_i + ((k-1)a+k) \sum_{j \neq i}^r n_j \right) \right)$$

$$= \frac{a}{4m^2} \left(-2k(a+1) \sum_{i=1}^r f_i + \sum_{i=1}^r n_i \left(2kf_i + ((k-1)a+k) \sum_{j \neq i}^r n_j \right) \right)$$

$$= \frac{a}{4m^2} \left(\sum_{i=1}^r 2kf_i(n_i - a - 1) + ((k-1)a+k) \sum_{i=1}^r \sum_{j \neq i}^r n_i n_j \right)$$

$$\geq \frac{a}{4m^2} \left(\sum_{i=1}^r 2kn_i(n_i - a - 1) + ((k-1)a+k) \sum_{i=1}^r \sum_{j \neq i}^r n_i n_j \right),$$

Here, $n_i \leq a-1$, so $n_i - a - 1 < 0$,
Hence, f_i increases
modularity difference
decreases and $f_i \leq n_i$

NP-Completeness (contd)

- Rearranging and using $a \geq 3k$

$$\begin{aligned}
 \Delta &\geq \frac{a}{4m^2} \sum_{i=1}^r n_i \left(2k(n_i - a - 1) \right. \\
 &\quad \left. + ((k - 1)a + k) \sum_{j \neq i}^r n_j \right) \\
 &= \frac{a}{4m^2} \sum_{i=1}^r n_i \left(-2k + ((k - 1)a - k) \sum_{j \neq i}^r n_j \right), \text{As } n_i + \sum_{j \neq i} n_j = a \\
 &\geq \frac{a}{4m^2} ((k - 1)a - 3k) \sum_{i=1}^r \sum_{j \neq i}^r n_i n_j \\
 &\geq \frac{3k^2}{4m^2} (3k - 6) \sum_{i=1}^r \sum_{j \neq i}^r n_i n_j .
 \end{aligned}$$

- Assuming $k > 2$, we see $\Delta > 0$

NP-Completeness (contd)

Lemma 4.2: In a maximum modularity clustering of $G(A)$, every cluster contains at most one of the cliques

H_1, H_2, \dots, H_k

- Cluster C contains $l > 1$ cliques completely and some element nodes a_j with $j \in J \subseteq \{1, 2, \dots, 3k\}$.
- Inside l cliques $la(a-1)/2$ edges are covered and degree sum is la^2 .
- For each element node a_j , la_j edges are covered and degree sum is $k \sum_{j \in J} a_j$.

NP-Completeness (contd)

- The contribution of \mathbf{C} to $q(\mathbf{C})$ is:

$$\frac{1}{m} \left(\frac{l}{2}a(a-1) + l \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(la^2 + k \sum_{j \in J} a_j \right)^2$$

- Clustering \mathbf{C}' in which \mathbf{C} is split into \mathbf{C}_1' and \mathbf{C}_2' .
- \mathbf{C}_1' completely contains a single clique \mathbf{H} .
- The contribution of \mathbf{C}_1' and \mathbf{C}_2' to $q(\mathbf{C}')$ is:

$$\frac{1}{m} \left(\frac{l}{2}a(a-1) + (l-1) \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(\left((l-1)a^2 + k \sum_{j \in J} a_j \right)^2 + a^4 \right)$$

NP-Completeness (contd)

- Considering the difference :

$$\begin{aligned}q(c') - q(c) &= -\frac{1}{m} \sum_{j \in J} a_j \\ &\quad + \frac{1}{4m^2} \left((2l-1)a^4 + 2ka^2 \sum_{j \in J} a_j - a^4 \right) \\ &= \frac{2(l-1)a^4 + 2ka^2 \sum_{j \in J} a_j}{4m^2} \\ &\quad - \frac{4m \sum_{j \in J} a_j}{4m^2} \\ &= \frac{2(l-1)a^4 - 2ka \sum_{j \in J} a_j}{4m^2} \\ &\geq \frac{9k^3}{2m^2} (9k-1) \\ &> 0,\end{aligned}$$

As $k > 0$ for all instance of 3-Partition

NP-Completeness (contd)

Lemma 4.3: In maximum modularity clustering of $G(A)$, there is no cluster composed of element nodes only.

- Element node v_i , corresponds to the element a_i , which is not a part of any clique cluster. The node v_i forms a singleton cluster $C = \{v_i\}$.
- C_{\min} is the clique cluster, for which the sum of degrees is minimal.
- C_{\min} contains all nodes from clique H , and some other element node a_j .

NP-Completeness (contd)

- The contribution of \mathbf{C} and \mathbf{C}_{\min} to $q(\mathbf{C})$ is:

$$\frac{1}{m} \left(\frac{a(a-1)}{2} + \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(\left(a^2 + k \sum_{j \in J} a_j \right)^2 + k^2 a_i^2 \right)$$

- Joining \mathbf{C} and \mathbf{C}_{\min} to form a new cluster \mathbf{C}' , now the contribution of \mathbf{C}' to $q(\mathbf{C}')$ is:

$$\frac{1}{m} \left(\frac{a(a-1)}{2} + a_i + \sum_{j \in J} a_j \right) - \frac{1}{4m^2} \left(a^2 + ka_i + k \sum_{j \in J} a_j \right)^2$$

NP-Completeness (contd)

Now,

$$\begin{aligned}q(C') - q(C) &= \frac{a_i}{m} - \frac{1}{4m^2} \left(2ka^2 a_i + 2k^2 a_i \sum_{j \in J} a_j \right) \\ &= \frac{1}{4m^2} \left(2ka(a+1)a_i - 2ka^2 a_i \right. \\ &\quad \left. - 2k^2 a_i \sum_{j \in J} a_j \right) \\ &= \frac{a_i}{4m^2} \left(2ka - 2k^2 \sum_{j \in J} a_j \right).\end{aligned}$$

As for C_{\min} .

$$\sum_{j \in J} a_j \leq \frac{1}{k} (a - a_i) < \frac{1}{k} a$$

Hence, $q(C') - q(C) > 0$

NP-Completeness (contd)

Theorem 4.4: Modularity is strongly NP-complete

- Polynomial time check $Modularity \in NP$
- Transformation of an instance of 3-Partition problem $A = \{a_1, a_2, \dots, a_{3k}\}$ to an instance of Modularity $(G(A), K(A))$.
- Clustering $G(A)$ follows the properties derived in previous lemmas.
- Any clustering yields $(k-1)a$ inter-cluster edges, so the edge coverage is:

$$\begin{aligned} \sum_{C \in \mathcal{C}} \frac{|E(C)|}{m} &= \frac{m - (k-1)a}{m} \\ &= 1 - \frac{2(k-1)a}{ka(a+1)} = 1 - \frac{2k-2}{k(a+1)} \end{aligned}$$

NP-Completeness (contd)

- The clustering with maximum modularity must minimize

$$\deg(C_1)^2 + \deg(C_2)^2 + \dots + \deg(C_k)^2$$

- This depends upon the distribution of element nodes, for the optimum case the distribution should be as even as possible.
- In the optimum case to each cluster assign element nodes that sums to $b = \frac{1}{k} a$
- In this case the sum of degrees of element nodes in each cluster is equal to $k \frac{1}{k} a = a$.
- This yields: $\deg(C_1)^2 + \dots + \deg(C_k)^2 \geq k(a^2 + a)^2 = ka^2(a + 1)^2$

NP-Completeness (contd)

- This yields: $\deg(C_1)^2 + \dots + \deg(C_k)^2 \geq k(a^2 + a)^2 = ka^2(a + 1)^2$
- Equality holds only if an assignment of \mathbf{b} is possible to every cluster.
- If the clustering \mathbf{C} with $q(\mathbf{C})$ of at least:

The clust $K(A) = 1 - \frac{2k - 2}{k(a + 1)} - \frac{ka^2(a + 1)^2}{k^2a^2(a + 1)^2} = \frac{(k - 1)(a - 1)}{k(a + 1)}$ \mathbf{k} clique clusters.

- The assignment of element nodes in \mathbf{k} clique clusters is also the solution to the 3-Partition problem.
- Hence, this choice of $\mathbf{K}(A)$ the instance $(\mathbf{G}(A), \mathbf{K}(A))$ of Modularity is satisfied only if the instance A of 3-Partition is satisfied, and vice-versa.

On Modularity Clustering (part 2)

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March 3, 2009

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Two Intrinsic Characteristics For Community Structure

Detection:

- No knowledge over the size of each community structure;
- No knowledge over the number of community structures of the input graph.

Definition

k -Modularity

Given a graph G and a number K , is there a clustering \mathcal{C} of G into exactly/at most k clusters, for which $q(\mathcal{C}) \geq K$?

Reduce from **Minimum Bisection for Cubic Graphs**.

Reduction

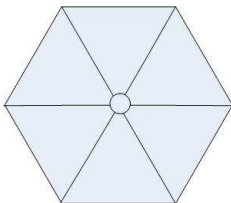
Minimum Bisection for Cubic Graphs(MB3)

Given a 3-regular graph G with n nodes and an integer c , is there a clustering into two clusters of $n/2$ nodes each such that it cuts at most c edges?

This problem is strongly NP-complete.

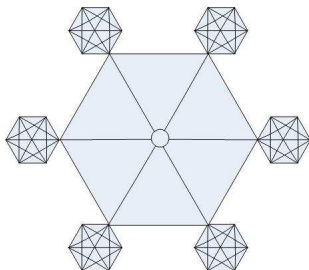
MB3 Instance

Construct a 2-Modularity instance from a MB3 Instance



2-Modularity Instance

Construct a 2-Modularity instance from a MB3 Instance



The following is to prove:

Give a bound K such that MB3 instance has a **bisection** cut of size at most c iff the corresponding graph has 2-modularity at least K .

Existence of such a clustering of two clusters?

Lemma 1

For every graph constructed from a MB3 instance, there exists a clustering $\mathcal{C} = \{C_1, C_2\}$ such that $q(\mathcal{C}) > 0$.

Proof:

- $C_1 = \text{cliq}(v)$ for some $v \in V$;
- $C_2 = V \setminus C_1$
- $q(\mathcal{C}) = 1 - \frac{3}{m} - \frac{(n(n-1)+3)^2 + ((n-1)(n(n-1)+3))^2}{4m^2} > 0$
 $(n \geq 4)$

$cliq(v)$ are all in one cluster?

Lemma 2

For every node $v \in V$ there exists a cluster $C \in \mathcal{C}^*$ such that $cliq(v) \subseteq C$.

Proof:

By contradiction, assume a clique $cliq(v)$ is split into two clusters:

- $\mathcal{C}' = \{C_1 \setminus cliq(v), C_2 \setminus cliq(v)\}$;
- $\Delta = q(\mathcal{C}') - q(\mathcal{C})$
 - $v \in C_2 \implies \Delta \geq 0$
 - $v \in C_1 \implies \Delta \geq 0$
- Clique moved into one cluster makes modularity larger.

Same size for each clusters in 2-Modularity Optimum?

Lemma 3

In C^* , each cluster contains exactly $n/2$ complete node cliques.

Proof:

By contradiction, assume a cluster C_1 has $l_1 \leq n/2 - 1$ cliques.

- $q(C^*) = \frac{m'}{m} - \frac{l_1^2(n(n-1)+3)^2}{4m^2} - \frac{(n-l_1)^2(n(n-1)+3)^2}{4m^2}$;
- C' := move one complete clique from C_2 to C_1 ; (lose at most 3 edges covered by inner-modularity)

$$q(C^*) = \frac{m'-3}{m} - \frac{(l_1+1)^2(n(n-1)+3)^2}{4m^2} - \frac{(n-l_1-1)^2(n(n-1)+3)^2}{4m^2}$$

- $q(C') \geq q(C)$
 (assume n to be even and $l_1 \leq \frac{n}{2} - 1$);

Strongly NP-complete

Strongly NP-completeness

A problem is said to be NP-hard in the strong sense (strongly NP-hard), if it remains so even when all of its numerical parameters are bounded by a polynomial in the length of the input.

Example: Bin Packing **VS** 0-1 Knapsack Problem

- Bin Packing: find a minimum integer B , such that n given items with relatively size a_1, a_2, \dots, a_n can be packed into B bins, where each bin has a given size V .
- 0-1 Knapsack Problem: given n items, each with value p_i and weight w_j for $i \in [1, n]$, maximize the total value of items that can be packed into a bag, on condition that the maximum weight carried in the bag is W . \iff can be solved by dynamic programming in $O(nW)$ time, note that, W is not polynomial of n . Otherwise, this is not NP-hard problem.

Strongly NP-complete

Theorem 1

2-Modularity is strongly NP-complete.

Proof:

- $K = \frac{1}{2} - \frac{c}{m}$;
- $\sum_{v \in C_i} \deg(v) = m$;
- if $q(C^*) \geq K = \frac{1}{2} - \frac{c}{m} = \frac{m-c}{m} - \frac{m^2}{4m^2} - \frac{m^2}{4m^2}$;
of inter-cluster edges can be **at most c**;
- Optimum $C^* \iff$ balanced partition cutting at most c edges.

Discussion

- 2-Modularity \leq_p k -Modularity?
- Corresponding algorithms?
- at least k clusters?? wired?

Contributions

- Algorithm by greedily merging clusters;
- Approximation ratio is at least 2.

Greedy Algorithm

Algorithm 1

Input: graph $G = (V, E)$

Output: clustering \mathcal{C} of G

$\mathcal{C} \leftarrow$ singletons;

symmetric matrix Δ with $\Delta_{i,j} = q(\mathcal{C}_{i,j}) - q(\mathcal{C})$;

▷ $\mathcal{C}_{i,j}$ is by merging clusters i, j ;

while $|\mathcal{C}| > 1$ and there exists $\Delta_{i,j} > 0$ **do**

merge clusters i and j where $\Delta_{i,j}$ is maximum;

▷ arbitrarily select one if multiple maximum exist;

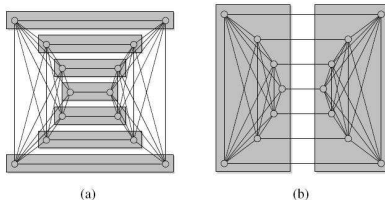
update matrix Δ ;

return clustering with the highest modularity

Worst Case

Theorem 2.1

No finite approximation factor for the greedy algorithm for finding clusterings with maximum modularity.



- worst case clustering: $q(C_a) = \frac{2}{n} - \frac{n}{2} \cdot \frac{4n^2}{n^4} = 0$
- one better clustering: $q(C_b) = \frac{n(n-2)}{n^2} - 2 \frac{4n^2}{16n^2} = \frac{1}{2} - \frac{2}{n} \leq opt$

Lower Bound

If re-mapping modularity interval from $[\frac{1}{2}, 1]$ to $[0, 1]$, the greedy algorithm in this instance can get an approximation ratio 2, but not for general case.

$$(q(C_a) = \frac{1}{3}; q(C_b) = \frac{2}{3})$$

Theorem 2.2

The approximation factor of the greedy algorithm is at least 2.

Optimality Results

Deal with two specific structures:

- Complete graph with n nodes – clique;
- Simple cycle with n nodes;

Both these two structures can be abstracted to d -regular graph

with $|E| = \frac{d|V|}{2}$

$$\rightarrow q(\mathcal{C}) = \frac{|E(\mathcal{C})|}{dn/2} - \frac{1}{n^2} \sum_{i=1}^k |C_i|^2$$

where $\mathcal{C} = \{C_1, \dots, C_k\}$

n -Clique

Theorem 3

Let k and n be integers, K_{kn} be the complete graph on $k \cdot n$ nodes and \mathcal{C} a clustering such that each cluster contains exactly n elements.

$$q(\mathcal{C}) = \left(-1 + \frac{1}{k}\right) \cdot \frac{1}{kn - 1}$$

Observations:

- $k > 1, n \rightarrow \infty, q(\mathcal{C}) \rightarrow 0^-$;
- $k = 1, q(\mathcal{C}) = 0$ is the global maximum;
- No further things??

n -Cycle (Simple 2-regular cycle with n nodes)

- Define $F(x) = 1 - q(\mathcal{C})$ where $x \in D^{(k)}$ is the vector of size k for k clusters; **Minimize** $F(x)$;
- $F(x) = \frac{k}{n} + \frac{1}{n^2} \sum_{i=1}^k x_i^2$ has global minimum at $x^* = \lfloor \frac{n}{k} \rfloor$ or $x^* = \lceil \frac{n}{k} \rceil$, i.e. evening cluster size decreases F .

n -Cycle (Simple 2-regular cycle with n nodes)

Based on these conclusions, we can have:

Lemma 2

Let C_n be a simple cycle with n nodes, $h : [1, \dots, n] \rightarrow \mathcal{R}$ a function defined as

$$h(x) := x \cdot n + n + \lfloor \frac{n}{x} \rfloor (2n - x \cdot (1 + \lfloor \frac{n}{x} \rfloor))$$

and k^* be the argument of the **global minimum** of h . Then every clustering of C_n with maximum modularity has k^* clusters.

Key:

$$h(k) = F(x^*)$$

n -Cycle

Theorem 4

Let n be an integer and C_n a simple cycle with n nodes. Then every clustering \mathcal{C} with maximum modularity has k cluster of almost equal size, where

$$k \in \left[\frac{n}{\sqrt{n} + \sqrt{n}} - 1, \frac{1}{2} + \sqrt{\frac{1}{4} + n} \right]$$

Proof:

- k is fixed by the distribution of cluster sizes with maximum modularity (even cluster size);
- with k outside this interval, function h is either monotonically increasing or decreasing;
- at most 3 possible values for large $n \iff k \in \left(\frac{n}{\sqrt{n}} - 1, \frac{1}{2} + \sqrt{\frac{1}{4} + n} \right]$

Any Questions



*<http://www.hardcore-stress->

[management.com/images/ManHoldingQuestionMarkSmallCropped.jpg](http://www.hardcore-stress-management.com/images/ManHoldingQuestionMarkSmallCropped.jpg)

