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Modularity of tree-like and random regular graphs

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Clustering algorithms for large networks typically use the modularity score to compare which partitions better represent modular structure in the data. Given a network, the modularity of a partition of the vertex set is a number in [0, 1) which measures the extent to which edge density is higher within parts than between parts; and the modularity of the network is the maximum modularity of any partition. We show that random cubic graphs usually have modularity in the interval (0.666, 0.804); and random *r*-regular graphs for large *r* usually have modularity $\Theta(1/\sqrt{r})$. Our results can give thresholds for the statistical significance of clustering found in large regular networks.

The modularity of cycles and low degree trees is known to be asymptotically 1. We extend these results to all graphs whose product of treewidth and maximum degree is much less than the number of edges. This shows for example that random planar graphs typically have modularity close to 1.

I. INTRODUCTION AND STATEMENT OF RESULTS

The greater availability of large network data in many fields has led to increasing interest in techniques to discover network structure. In the analysis of these networks, clusters or communities found using modularity optimisation have become a focus of scientific study. Thus we need a test to determine the statistical significance of observed community structure [1]. We give bounds in Table I which the modularity of random regular graphs will typically satisfy. This gives the best known thresholds for statistical significance of modular structure in regular networks.

The popularity of modularity based clustering techniques and the link to the Potts model in statistical physics [2] have prompted much research into behaviour of the modularity function on families of graphs. The asymptotic modularity of each of the following graph classes was shown to be maximal; cycles [3], low degree trees [4, 5] and lattices [6]. We extend the first three results in Theorem 3 which shows maximal modularity for graphs whose product of tree-width and maximum degree is much less than the number of edges. This includes random planar graphs.

These structural results on graph families are interesting both to examine the clusters in graph classes and to judge the effectiveness of the modularity function in identifying modular structure.

A. Modularity function

The definition of modularity was first introduced by Newman and Girvan in [7]. Most popular algorithms used to search for clusterings on large datasets are based on finding partitions with high modularity [8]. It has been applied to identify clusters of neurons in the brain [9] and groups in social networks [10]. See [11] for a survey on community detection including modularity based methods.

The modularity function is designed to score partitions highly when most edges fall within the parts and penalise partitions with very few or very big parts. These two objectives are encoded as the *edge contribution* $q_{\mathcal{A}}^{E}(G)$, and *degree tax* $q_{\mathcal{A}}^{D}(G)$, in the modularity of a vertex partition \mathcal{A} of G. Denote the number of edges in the subgraph induced by vertex set A by e(A), and the sum of the degrees (in the whole graph G) of the vertices in Aby degsum(A). For a graph with $m \geq 1$ edges, we set

$$q_{\mathcal{A}}^{E}(G) = \frac{1}{m} \sum_{A \in \mathcal{A}} e(A)$$
$$q_{\mathcal{A}}^{D}(G) = \frac{1}{4m^{2}} \sum_{A \in \mathcal{A}} \operatorname{degsum}(A)^{2}$$
$$q_{\mathcal{A}}(G) = q_{\mathcal{A}}^{E}(G) - q_{\mathcal{A}}^{D}(G).$$

The *(maximum) modularity* $q^*(G)$ of a graph G is then the maximum value of $q_{\mathcal{A}}(G)$ over all partitions, that is

$$q^*(G) = \max_{\mathcal{A}} q_{\mathcal{A}}(G).$$

B. Random regular graphs

How should we study the statistical significance of clusters in regular networks? There has been recent interest in estimating the modularity of random graphs [1, 6, 12]. In order to tell if a given partition shows statistically significant clustering in a network it is natural to compare

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r =	3	4	5	6	7	8	9	10	11	12
$q^*(G_r) >$	0.666	0.500	0.400	0.333	0.285	0.250	0.226	0.214	0.204	0.196
$q^*(G_r) <$	0.804	0.684	0.603	0.544	0.499	0.463	0.433	0.408	0.388	0.370

TABLE I. The upper and lower bounds for the maximum modularity of random regular graphs proven in Theorem 1.

the modularity score to that of a corresponding random graph model. We give results which bound the modularity of random r-regular graphs. In our first main theorem, Theorem 1 (which appeared in [13]), we consider small values of r; and improve results in [14].

When an event holds with probability tending to 1 as $n \to \infty$ we say that it holds with high probability (whp).

Theorem 1. For r = 3, ..., 12, the modularity of a random r-regular graph G_r why lies in the range indicated in Table I.

Our second main theorem shows that for r large the modularity of the random r-regular graph G_r is $\Theta(1/\sqrt{r})$ whp. The upper bound below on $q^*(G_r)$ is given also in [15].

Theorem 2. There is a constant c > 0 such that, for each $r \ge 2$ and each r-regular graph G on sufficiently many vertices, we have

$$q^*(G) \ge c/\sqrt{r}.$$

There is an r_0 such that for each $r \ge r_0$

$$q^*(G_r) \le 2/\sqrt{r} + 1/r \quad whp$$

C. Tree width and maximum degree

Bagrow makes a study of the modularity of some trees and tree-like graphs in [4]. He shows Galton-Watson trees and k-ary trees have modularity tending to one. In [5] it is proven that any tree with maximum degree $\Delta(G) = o(n^{1/5})$ has asymptotic modularity one. Our results show this extends to all trees with $\Delta(G) = o(n)$. We further extend these results by showing this high modularity of low degree trees extends to those graphs which are tree-like, i.e. have low treewidth. This forms Theorem 3.

Let us recall the definition of treewidth: see [16] for a survey. A *tree-decomposition* of a graph G = (V, E)is a pair consisting of a tree T = (I, F) and a family $(X_i : i \in I)$ of subsets of V ('bags'), one for each node of T, such that

1. $\cup_{i \in I} X_i = V$

- 2. $\forall vw \in E, \exists i \in I \text{ such that } v, w \in X_i.$
- 3. $\forall i, j, k \in I$: if j is on the path between i and k in T, then $X_i \cap X_k \subseteq X_j$.

The width of a tree decomposition is $\max_{i \in I} |X_i| - 1$; and the *treewidth* of a graph G is the minimum width over all tree decompositions of G.

The following result is our key tool for lower bounding q^* for graphs with small treewidth and maximum degree. In particular, Corollary 5 gives the lower bounds on $q^*(G_r)$ for $r = 3, \ldots, 8$ in Theorem 1. (These lower bounds were originally proved in [14] using a Hamilton cycle construction.)

Theorem 3. Let G be a graph with $m \ge 1$ edges and maximum degree $\Delta = \Delta(G)$, and let E' be a set of edges such that $tw(G \setminus E') \le t$. Then the modularity $q^*(G)$ satisfies

$$q^*(G) \ge 1 - 2((t+1)\Delta/m)^{1/2} - |E'|/m.$$

Consider graphs G with bounded degree and bounded treewidth, for example cycles. The last result (with $E' = \emptyset$) shows that if G has m edges then $q^*(G) \ge 1 - O(m^{-\frac{1}{2}})$. This lower bound is tight for connected graphs.

Proposition 4. If G is a connected graph with $m \ge 1$ edges then $q^*(G) \le 1 - \frac{1}{\sqrt{m}}$.

We next give two corollaries of Theorem 3. The first gives a lower bound on the modularity of any r-regular graph.

Corollary 5. Let $r \ge 2$ and let G be any r-regular graph on n vertices. Then $q^*(G) \ge 2/r - 2\sqrt{6/n}$.

We shall deduce this result from Theorem 3 after proving that theorem. We see that every *r*-regular graph has modularity at least $q^*(G) \ge 2/r - o(1)$. Thus the lower bounds proven to hold whp for random *r*-regular graphs in [14] actually hold for all large *r*-regular graphs. Note that for large *r* the lower bound here is much weaker than that in the first part of Theorem 2.

Our second corollary of Theorem 3 is immediate.

Corollary 6. For m = 1, 2, ... let G_m be a graph with m edges. If $tw(G_m) \cdot \Delta(G_m) = o(m)$ then $q^*(G_m) \to 1$ as $m \to \infty$.

This result is best possible, in that we cannot replace o(m) by O(m): here are two examples.

(a) If G is the star $K_{1,m}$ (with treewidth 1 and maximum degree m) then $tw(G) \cdot \Delta(G) = 1 \cdot m = m$ and $q^*(G) = 0$ [5].

(b) If G is the random cubic graph on n vertices (so m = 3n/2) then $tw(G) \cdot \Delta(G) = 3tw(G) = O(m)$. However by Theorem 1 $q^*(G) \leq 0.804$ whp.

Corollary 6 shows that random planar graphs, and more generally random graphs on surfaces, whp have modularity near 1. For a given surface S, let the graph $G_S(n)$ be chosen uniformly from all labelled *n*-vertex graphs which embed in S (without crossing edges). Then G_S has $tw(G_S) = O(\sqrt{n})$ by [17], [18] and whp it has maximum degree $\Delta(G_S) = O(\log n)$ [19] and $\Theta(n)$ edges, so whp

$$q^*(G_S(n)) \ge 1 - O((\log n)^{\frac{1}{2}}/n^{\frac{1}{4}}) = 1 - o(1).$$

II. PROOFS: LOWER BOUNDS ON MODULARITY

A. Proof of Theorem 3

To prove Theorem 3 (the 'treewidth lower bound') we need one lemma.

Lemma 7. Let the graph G have m edges, maximum degree d and set $E' \subset E(G)$ such that $tw(G \setminus E') = t$. Let s be an integer such that $d < s \leq 2m - d$. By deleting the edges incident with at most t+1 vertices, we can find a partition $V(G) = V_0 \cup \cdots \cup V_{k-1}$ into $k \geq 3$ parts with no cross-edges in $G \setminus E'$ such that $degsum(V_0) \leq 2m - s$ and $degsum(V_i) < s$ for each $i = 1, \ldots, k - 1$.

Proof. The first step is to delete the edges in E', writing $H = G \setminus E'$. We introduce a weight function to remember the positions of the edges in E'. For each vertex $v \in H$ define $w(v) = deg_G(v)$ and the weight of a vertex set $w(V) = \sum_{v \in V} w(v)$.

The proof will take a tree-decomposition of H, choose one bag X_i , and delete all edges of H incident to the vertices in X_i . Observe we can guarantee a tree decomposition T of width t such that if ij is an edge of T then $|X_i \triangle X_j| \leq 1$; and further each leaf i of T has bag X_i of size 1. Fix such a tree decomposition, and fix a leaf to be the root vertex.

Recall that deleting any edge in a tree leaves exactly two connected components. For any edge e in T let T_e denote the non-root component of $T \setminus e$; let V_e be the set of vertices contained in the bags of T_e ; and let $d_e = \text{degsum}(V_e)$, the sum of the degrees in G of these vertices. If $d_e < s$, then orient e toward the root vertex; otherwise, orient e away from the root vertex.

At least one node in T has out-degree zero. Fix such a node i. Notice i is not the root (since $s \leq 2m - d$), and i is not a leaf (since then $|X_i| = 1$ and so degsum $(X_i) \leq d < s$). We shall delete the edges of Hincident with the vertices in the bag X_i . Thus we delete at most (t+1)d edges. Let e be the edge incident with iwhich lies on the path from the root vertex to node i. Let $V_0 = V(G) \setminus V_e$. Since degsum $(V_e) \geq s$ we have $\operatorname{degsum}(V_0) \le 2m - s.$

Since *i* is not a leaf in *T*, other than its neighbour along edge *e*, *i* has neighbours j_1, \ldots, j_k for some $k \ge 1$. If there is one such neighbour, let $V_1 = V_{ij_1}$ and $V_2 = X_i \setminus V_1$, so degsum $(V_1) < s$ (since the edge $j_1 i$ is oriented towards *i*) and degsum $(V_2) \le d < s$ (since $|V_2| = 1$). Similarly if there are multiple neighbours, let $V_1 = V_{ij_1}, \ldots, V_k =$ V_{ij_k} , and $V_{k+1} = X_i \setminus (V_1 \cup \ldots \cup V_k)$, so degsum $(V_i) < s$ for each *i*.

Proof of Theorem 3

Write d for Δ . Since $q^*(G) \geq 0$ for any graph G we need only prove the case where $m \geq 4(t+1)d$. Let $s = \lceil 2((t+1)dm)^{\frac{1}{2}} \rceil$. Note that $s \geq 4(t+1)d$.

Set $\tilde{G} = G$ and $\tilde{m} = e(\tilde{G})$. Observe that s > d. As long as $2\tilde{m} \ge s + d$ we use the last lemma repeatedly to 'break off parts' V_1, V_2, \ldots and replace \tilde{G} by its induced subgraph on V_0 , where degsum $(V_0) \le 2\tilde{m} - s$. After $j \le 2m/s - 1$ steps we have $2\tilde{m} < s + d$. At this stage we have lost at most j(t + 1)d edges, and each of the parts 'broken off' from G has degree sum $\le s - 1$.

We claim we can complete this to a partition of V(G) such that each part has degree sum at most s-1 and the number of cross-edges in $G \setminus E'$ is at most $\frac{2m}{s}(t+1)d$. If $2\tilde{m} \leq s-1$ we are already done; so consider the other case, when $s \leq 2\tilde{m} < s+d$. Now let s' = s-d, and note that s' > d. We can apply the lemma with s' to complete the proof of the claim, since

$$2\tilde{m} - s' < s + d - (s - d) = 2d \le s$$

Note that $0 \le x_i \le s - 1$ and $\sum_i x_i \le 2m$ together imply $\sum_i x_i^2 \le 2m(s-1)$, and so finally, by the claim and our choice of s a

$$\begin{split} 1 - |E'|/m - q^*(G) &\leq \frac{1}{m} \frac{2m(t+1)d}{s} + \frac{2m(s-1)}{4m^2} \\ &= \frac{2(t+1)d}{s} + \frac{s-1}{2m} \\ &\leq \frac{2(t+1)d}{2((t+1)dm)^{\frac{1}{2}}} + \frac{2((t+1)dm)^{\frac{1}{2}}}{2m} \\ &= 2\left(\frac{(t+1)d}{m}\right)^{\frac{1}{2}}, \end{split}$$

and this completes the proof.

Proof of Corollary 5 For each connected component H of G do the following. In H choose a spanning tree together with one extra edge (observe that H is not a tree since $r \geq 2$), and let E'_H be the set of edges not chosen.

Each unicyclic graph has tree-width 2, so $tw(H \setminus E'_H) = 2$. Define $E' = \bigcup_H E'_H$, and note that $tw(G \setminus E') = 2$ and |E'| = m - n, where e(G) = m = rn/2. Hence by Theorem 3

$$q^*(G) \ge 1 - 2(\frac{3r}{m})^{\frac{1}{2}} - (1 - \frac{n}{m}) = \frac{2}{r} - 2(\frac{6}{n})^{\frac{1}{2}}$$

as required.

B. Bisection width

Define the bisection width bw(G) of a graph G to be

$$bw(G) = \min_{|U| = \lfloor \frac{n}{2} \rfloor} e(U, \overline{U})$$

where the minimum is over all sets U of $\lfloor \frac{n}{2} \rfloor$ vertices, and \overline{U} denotes $V(G) \backslash U$. It is easy to check that for an *r*-regular graph G,

$$q^*(G) \ge \frac{1}{2} - \frac{2bw(G)}{rn} - \frac{1}{2r^2n^2}$$

where we do not need the last (small) term if n is even.

It was shown in [20] that whp the bisection width of a random 12-regular graph is at most 1.823. This implies that whp $q^*(G_{12}) > 0.196$, as given in Theorem 1 (Table I). Similar calculations apply for r = 9, 10, 11 which have bisection widths at most 1.2317, 1.4278, 1.624 respectively [20]. (We noted earlier that Corollary 5 gives the lower bounds on $q^*(G_r)$ for $r = 3, \ldots, 8$ in Theorem 1: currently known results on bisection width do not improve on the 2/r lower bound.)

Now consider large r. By Theorem 1.1 of Alon [21], there is a constant c > 0 such that, for all r and all sufficiently large r-regular graphs

$$bw(G)/n \le r/4 - c\sqrt{r}.$$

Hence for each r-regular graph G with sufficiently many vertices we have

$$q^*(G) \ge c/\sqrt{r}.$$

III. PROOFS: UPPER BOUNDS ON MODULARITY

First let us give a short and easy proof.

Proof of Proposition 4

Recall that G is a connected graph with $m \ge 1$ edges. Consider a partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ of V(G) into k parts, where A_j contains m_j edges (and so $m = \sum_j m_j$). Since G is connected, there must be at least k - 1 cross edges; and

$$q^D_{\mathcal{A}}(G) = (1/m^2) \sum_j m_j^2 \ge 1/k$$

since $(1/k) \sum_{j} m_{j}^{2} \ge (m/k)^{2}$ by convexity. Hence

$$q_{\mathcal{A}}(G) \le 1 - \frac{k-1}{m} - \frac{1}{k} \le 1 + \frac{1}{m} - \frac{2}{\sqrt{m}},$$

so $q^*(G) \le 1 - \frac{1}{\sqrt{m}}$, as required.

We next introduce some parameters for regular graphs, related to expansion or homogeneity. For a non-empty set S of vertices in a graph G, let $\bar{d}(S)$ denote the average degree of the induced subgraph on S, so $\bar{d}(S) = \frac{2e(S)}{|S|}$. Now let $r \ge 2$ and suppose that G is r-regular and has n vertices. Let

$$\beta = \beta(G) = \max_{|S| \le n/2} \left(\frac{\bar{d}(S)}{r} - \frac{|S|}{n}\right)$$

where the maximum is over all non-empty sets S of at most n/2 vertices. We claim that

$$\frac{\bar{d}(S)}{r} - \frac{|S|}{n} \le \beta \tag{1}$$

for all non-empty sets S of vertices.

To establish this claim, let S be a set of vertices with $|S|/n = u > \frac{1}{2}$. We must show that $\frac{\bar{d}(S)}{r} - u \leq \beta$. Since $2e(S) = r|S| - e(S, \bar{S})$ and similarly $2e(\bar{S}) = r(n - |S|) - e(S, \bar{S})$, we have

$$2e(S) = 2e(\bar{S}) + run - r(1-u)n = 2e(\bar{S}) + (2u-1)rn.$$

Hence

$$\frac{\bar{d}(S)}{r} - u = \frac{2e(S)}{run} - u$$
$$= \frac{2e(\bar{S}) + (2u - 1)rn}{run} - u$$
$$\leq \frac{r(1 - u)n(1 - u + \beta) + (2u - 1)rn}{run} - u$$
$$= \frac{(1 - u)\beta}{u} \leq \beta$$

since $u \ge \frac{1}{2}$. This completes the proof of claim (1).

Following the notation of [22], for $0 < u \leq \frac{1}{2}$ we define the *u*-edge expansion $i_u(G)$ of an *n*-vertex graph G by setting

$$i_u(G) = \min_{|U| \le un} \frac{e(U,\bar{U})}{|U|}$$

where the minimum is over non-empty sets U of at most un vertices (and the value is taken to be ∞ if un < 1). Observe that $i_{1/2}(G)$ is the usual edge expansion or isoperimetric number of G. Also, set

$$\alpha = \alpha(G) = \min_{0 < u \le \frac{1}{2}} (u + i_u(G)/r).$$

We claim that

$$\alpha + \beta = 1. \tag{2}$$

To establish claim (2) we may argue much as above. Since $run = 2e(S) + e(S, \overline{S})$ we have

$$2e(S) - ru^{2}n = ru(1 - u)n - e(S, \bar{S}),$$

and so

$$\frac{\bar{d}(G)}{r} - u = 1 - (u + \frac{e(S,\bar{S})}{r|S|}).$$

Hence $\beta = 1 - \alpha'$ where

$$\alpha' = \min_{|S| \le n/2} \left(u + \frac{e(S,\bar{S})}{r|S|} \right).$$

But it is easy to see that $\alpha' = \alpha$, which completes the proof of claim (2).

Given an *n*-vertex graph G with eigenvalues $\lambda_1 \geq .. \geq \lambda_n$, let

$$\lambda = \lambda(G) = \max_{i>1} |\lambda_i| \quad (= \max\{|\lambda_2|, |\lambda_n|\})$$

(as for example in section 9.2 of Alon and Spencer [23]).

Lemma 8. Let G be an r-regular graph. Then

$$q^*(G) \le \beta \le \lambda/r.$$

Proof. Let G have n vertices, let S be a non-empty set of vertices, and let u = |S|/n. By Corollary 9.2.6 of Alon and Spencer [23] (see also Lemma 2.3 of Alon and Chung [24])

$$|e(S) - \frac{1}{2}ru^2n| \le \frac{1}{2}\lambda un$$

Hence

$$\left|\frac{\bar{d}(S)}{r} - u\right| = \frac{|e(S) - \frac{1}{2}ru^2n|}{\frac{1}{2}run} \le \lambda/r;$$

and so $\beta \leq \lambda/r$. Now consider any partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ of V(G). Letting $u_j = |A_j|/n$, and using (1) if some $u_j > \frac{1}{2}$, we have

$$q_{\mathcal{A}}(G) = \sum_{j} \left(\frac{2e(A_j)}{rn} - \frac{(u_j rn)^2}{(rn)^2} \right)$$
$$= \sum_{j} u_j \left(\frac{\bar{d}(A_j)}{r} - u_j \right)$$
$$\leq \beta \sum_{j} u_j = \beta.$$

Hence $q^*(G) \leq \beta$, as required.

Proof of upper bounds in Theorem 1

Detailed results which give a lower bound on $i_u(G)$ as a function of u were given in [22], where a function $f_r(u)$ is defined and it is shown that, for a random r-regular graph G_r , whp $i_u(G_r) > f_r(u)$. These results imply that whp for a random cubic graph G_3 , the inequality $u + i_u(G_3)/3 > 0.196$ holds for all $u \leq 1/2$; that is, $\alpha(G_3) > 0.196$ and so $\beta(G) < 0.804$ by (2). But now Lemma 8 shows that whp $q^*(G_3) < 0.804$. Similarly, calculating $f_r(u)$ for other values of r yields the upper bounds given in Table I.

Proof of upper bounds in Theorem 2

Let G_r be a random r-regular graph (with r fixed). Friedman [25] showed that whp $\lambda(G_r) \leq 2\sqrt{r-1} + o(1)$ (where the o(1) is as $r \to \infty$). Thus we see from the last lemma that whp $q^*(G_r) \leq 2r^{-\frac{1}{2}} + o(1/r)$.



FIG. 1. Theorem 1 says that the modularity of a random regular graph G_r whp lies in the interval shown.

IV. CONCLUDING REMARKS

Two main contributions of this paper are (a) the numerical bounds for the modularity of random regular graphs, which can be used to investigate the significance of observed clustering; and (b) showing the high modularity in certain graph families, such as low degree treelike graphs and random planar graphs.

We saw classes of graphs for which the modularity is bounded strictly away from 0 and 1, or for which the modularity approaches 0 or 1. For fixed r, random r-regular graphs have modularity bounded strictly away from 0 and 1 whp, and for large r the modularity approaches 0 whp, whereas random planar graphs and graphs with small treewidth and small maximum degree have modularity approaching 1.

Simulations suggest that the modularity of the random cubic graph G_3 is close to 2/3 whp. Is this the limit?

Conjecture 9. $q^*(G_3) = 2/3 + o(1)$ whp.

Corollary 5 shows that the modularity of any large cubic graph is at least 2/3 - o(1), so if Conjecture 9 is correct then the random cubic graph is asymptotically an extremal example.

In a forthcoming paper [26] we note that lattices can be considered as a special case of graphs which embed in space with small ratio between maximum edge length and minimum vertex separation (that is, 'small distortion'), and we show that all large graphs with this property have high modularity.

In a forthcoming companion paper [12] to the present paper, we investigate the modularity of Erdős-Rényi random graphs, and use Theorem 3 to give a lower bound on the modularity in the super-critical regime.

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