Modularity of Networks

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Abstract

Modularity is a quality function on partitions of a network which may be used to identify highly clustered components. It is commonly used to analyse large real networks, for example in social networks and protein discovery to find communities and related proteins respectively. Given a graph G, the modularity of a partition of the vertex set measures the extent to which edge density is higher within parts than between parts, and the maximum modularity $q^*(G)$ of G (where $0 \leq q^*(G) < 1$) is the maximum modularity of a partition of $V(G)$. In essence, modularity allows us to feed in large sets of data, and output a vertex partition with an associated score.

Knowledge of the maximum modularity of random graphs is important to determine the statistical significance of the maximum modularity found on a real network. This thesis establishes numerical bounds on the likely maximum modularity for random regular graphs. The modularity of a random cubic network is shown to be whp in the interval (0.66, 0.81). This result has practical applications. It establishes that a large cubic network with modularity greater than 0.81 has a statistically significant clustering structure.

The evolution of the maximum modularity of Erdős-Rényi random graphs as the edge probability increases is investigated. Three different phases of the likely maximum modularity are found. For $np = 1 + o(1)$ the maximum modularity is $1 + o(1)$ whp and for $np \to \infty$ the maximum modularity is $o(1)$ whp. For $np = c$ with $c > 1$ a constant, functions are constructed with $0 < a(c) < b(c) < 1$ and $b(c) \to 0$ as $c \to \infty$ such that whp the maximum modularity is bounded between these functions. Concentration of the maximum modularity about its expectation and structural properties of any optimal partition are also established.

Finding the maximum modularity of graph classes helps us understand the behaviour of the modularity function. We study trees, lattices and related graphs. The maximum modularity of a large k-ary tree was shown to be near 1 by Bagrow [2]. This was extended to trees with maximal degree $o(n^{1/5})$ in [16]. This thesis further extends the result to any tree with maximal degree $o(n)$. Indeed it is shown that the maximum modularity will tend to 1 for any graph where the product of the treewidth and the maximal degree is much less than the number of edges. This shows random planar graphs typically have modularity $1 + o(1)$.

Lower bounds were given in Guimerà et al. [27] for the maximum modularity of complete sections of the integer lattice and for lattices with extra axis aligned edges included. The maximum modularity of any subgraph of this lattice is shown to be at least the same order of magnitude in the number of edges. This generalises to any graph which can be embedded in Euclidean space such that no edge is too long and no two vertices fall too close together.

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My acknowledgements go to the Statistics Department for funding my DPhil. I want to thank Dan Král' for introducing me to graph limits and for my research stay at Warwick University, and Brendan McKay for the introduction to probabilistic combinatorics itself.

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In Oxford I go on to thank the Balliol graduate community for many spirited discussions and ceilidhs, my fellow kayakers of OUCKC esp. Anja, Hannah, Giacomo, Matt, Seiko and Tom H, housemates esp. Bahar, Brendan and Kati, the Balliol rowing crew esp. Clarissa, Mima and Mira. Also to Elsje, Gabi, Jakub and Martin who defy such categorisation.

Lastly I thank my Mum, Dad, sister and extended family for their unsurpassable welcomes on my infrequent trips home à la *drinking white wine in the sun*, for their visits to the UK and even a technicolour quilt to help me through my first and subsequent winters here.

Statement of originality

All work is my own developed in collaboration with my supervisor Colin McDiarmid.

To my Mum, Dad and sister,

Contents

Chapter 1

Introductory remarks

This chapter serves many purposes. We will introduce the notion of modularity and survey and clarify past results. We also prove several simple results to help us understand the basic behaviour of modularity as well as preparatory lemmas in readiness for later parts of the thesis.

After this long introductory chapter, the thesis falls into two parts. Chapters 2-4 give new deterministic results on modularity and Chapters 5 and 6 give new results on modularity for random graphs. A summary of the contribution of the thesis as well as an outline is given on p18.

1.1 Introduction to modularity

We give a gentle introduction to the modularity function and describe its use in network science and relationship to statistical physics and graph theory. This section ends with a summary of the contribution of the thesis and a structural outline.

1.1.1 Modularity function

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 have become a focus of scientific study.

The focus of this thesis is modularity, a measure of how clumped a network is into communities. Introduced by Newman and Girvan in 2004 [50], modularity now forms the backbone of the most popular algorithms to cluster large real networks [38]. There are many applications including protein discovery, identifying connections between websites and mapping the onset of schizophrenia on neuron clusters in the brain [1]. Modularity has been used to cluster networks of 10 million nodes [59]. Its widespread use and empirical success in finding communities in networks makes modularity an important function to understand mathematically. See [23] and [54] for surveys on the use of modularity for community detection in networks.

Suppose in your graph you have a number of disjoint groups of vertices which are highly connected within themselves but not to the rest of the graph. Suppose also that you don't know the sizes of these groups. Weighting candidate partitions by the modularity function is designed to identify these groups.

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. The formula of modularity naturally splits into two expressions each performing one of these functions. We will often analyse these two parts of the formula for modularity separately and so we define the *edge contribution* and *degree tax* of the modularity function.

The definition requires a little notation. The input to our function is a simple graph G with $m \geq 1$ edges and a partition $\mathcal{A}$ of the vertices of G. For a subset of vertices A, we denote by $e(A)$ the number of edges in the subgraph induced on A and by $\mathrm{ds}(A)$ the sum of the degrees in G of all vertices in A (see p21 for detailed notation).

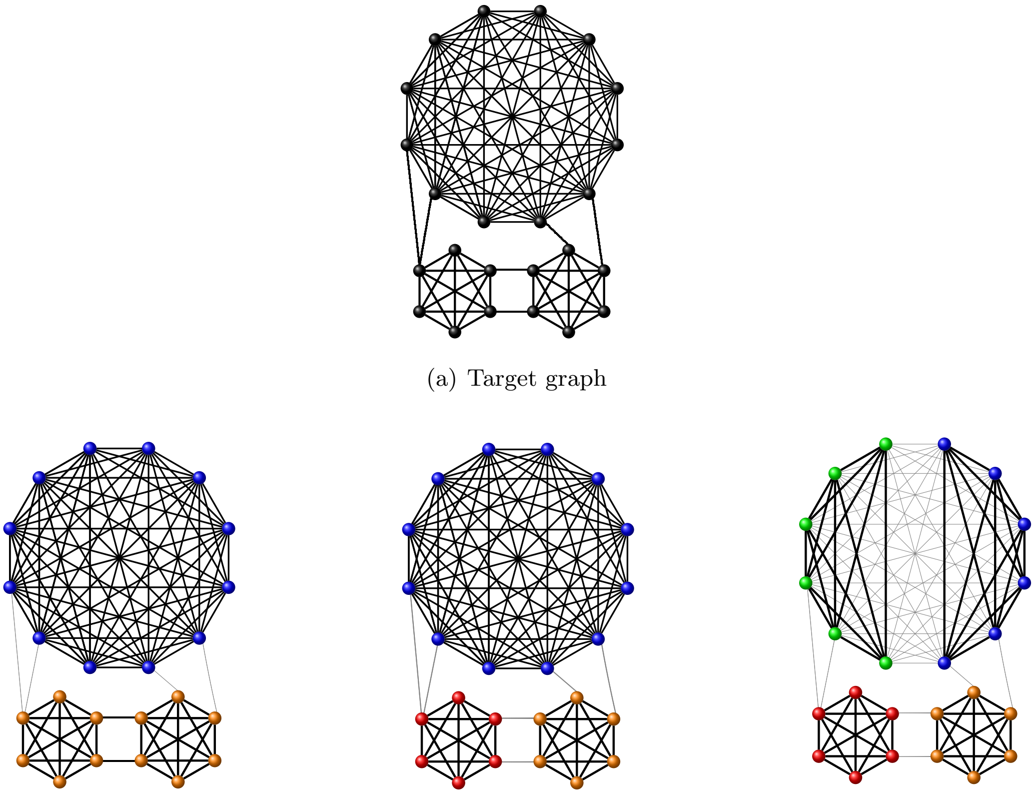
Definition 1.1.1. *Let G be a graph with $m \geq 1$ edges and $\mathcal{A}$ a vertex partition of G. Then define the edge contribution $q^E_{\mathcal{A}}(G)$, degree tax $q^D_{\mathcal{A}}(G)$, and modularity $q_{\mathcal{A}}(G)$:*

$$q^E_{\mathcal{A}}(G) = \frac{1}{m} \sum_{A \in \mathcal{A}} e(A), \qquad q^D_{\mathcal{A}}(G) = \frac{1}{4m^2} \sum_{A \in \mathcal{A}} \mathrm{ds}(A)^2,$$
$$q_{\mathcal{A}}(G) = q^E_{\mathcal{A}}(G) - q^D_{\mathcal{A}}(G).$$

The maximum modularity*, $q^*(G)$, of a graph G is the maximum over all partitions,*

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

Observe that $0 \leq q^*(G) < 1$ for any graph G with $m \geq 1$ edges. The upper bound is easy because the edge contribution is at most 1, and the degree tax is positive which bounds us strictly below 1. For the lower bound, take the vertex partition which places all vertices in



(a) Target graph

(b) $\mathcal{A}_1$

(c) $\mathcal{A}_2$

(d) $\mathcal{A}_3$

$q^E_{\mathcal{A}_1} \approx 0.96, \quad q^D_{\mathcal{A}_1} \approx 0.56$

$q_{\mathcal{A}_1} \approx 0.40$

$q^E_{\mathcal{A}_2} \approx 0.94, \quad q^D_{\mathcal{A}_2} = 0.5$

$q_{\mathcal{A}_2} \approx 0.44$

$q^E_{\mathcal{A}_3} \approx 0.59, \quad q^D_{\mathcal{A}_3} \approx 0.28$

$q_{\mathcal{A}_3} \approx 0.31$

Figure 1.1: Modularity calculations of three candidate partitions.

the same part, i.e. $\mathcal{A} = \{V\}$, then the edge contribution and degree tax are both exactly 1 and so $q_{\{V\}}(G) = 0$. It can also be shown for any partition $\mathcal{A}$ that $q_{\mathcal{A}}(G) \in [-1/2, 1)$ [13].

As an example, consider the toy graph on 24 vertices and 102 edges shown in Figure 1.1(a). The edge contribution, degree tax and modularity of three different candidate vertex partitions (partitions indicated by vertex colours) for this toy graph are computed in Figure 1.1(b)-(d).

1.1.2 Relation to statistical physics

It was noted in [27], that a partition with maximal modularity corresponds to a distribution of spin states which has the lowest energy under some parameters of the Potts model placing modularity as a special case of a larger system. This connection was also detailed in [56]. We think this provides a good perspective on modularity and so we rederive the result.

First let us introduce the Potts model. For a given graph on n vertices, the q-state Potts model defines an energy for each assignment σ of vertices to the different states $1, \ldots, q$ given by,

$$E_\sigma(G, J) = \exp\big(- \sum_{u,v \in V(G)} J_{uv} 1_{\sigma(u)=\sigma(v)} \big),$$

where $1_{\sigma(u)=\sigma(v)}$ is the indicator for the event that u, v are assigned the same state and J is an $n \times n$ matrix referred to as the coupling matrix [56].[1] The coupling matrix is tuned to suit the situation. If the value of $J_{uv} > 0$ then the Potts model is said to have a *ferromagnetic* coupling between vertices u and v and likewise, if $J_{uv} < 0$ we say there is an *anti-ferromagnetic* coupling between vertices u and v.

We will demonstrate that for a particular choice of the coupling matrix J the assignment(s) σ which yield(s) the lowest energy of G in a q-state Potts will correspond to the partition(s) $\mathcal{A}$ which has the highest modularity of any vertex partition with q parts.

To show that such a choice of coupling matrix J exists we rewrite modularity in a particular way. Recall the modularity $q_\mathcal{A}(G)$ gives a score to a particular vertex partition $\mathcal{A} = \{A_1, \ldots, A_q\}$ of a graph G. Then, as in Definition 1.1.1,

$$q_\mathcal{A}(G) = \sum_{A_i \in \mathcal{A}} \frac{e(A_i)}{m} - \frac{\mathrm{ds}(A_i)^2}{4m^2}.$$

Observe that our vertex partition $\mathcal{A}$ induces a map from vertices in the graph to parts in our vertex partition. If $v \in A_i$ we write this map as $\sigma_\mathcal{A}(v) = i$. We have denoted the map σ in homage to statistical physics – in the language of the Potts model you would say σ is an assignment of vertices to states.

This allows us to rewrite the expression for modularity in terms of indicator variables. Note $1_{\sigma_\mathcal{A}(v)=\sigma_\mathcal{A}(u)}$ indicates the event that vertices u, v are assigned to the same part in $\mathcal{A}$ and $1_{uv \in E}$ indicates the event that uv is in the edge set of G.

[1] There is sometimes an extra term to model an external magnetic field, see [56].

$$
\begin{aligned}
q_{\mathcal{A}}(G) &= \frac{1}{2m} \sum_{A_i \in \mathcal{A}} 2e(A_i) - \frac{\mathrm{ds}(A_i)^2}{2m} \\
&= \frac{1}{2m} \sum_{A_i \in \mathcal{A}} \left(\sum_{u,v \in A_i} 1_{uv \in E} - \frac{\deg(u)\deg(v)}{2m} \right) \\
&= \frac{1}{2m} \left(\sum_{u,v \in V(G)} 1_{uv \in E} - \frac{\deg(u)\deg(v)}{2m} \right) 1_{\sigma_{\mathcal{A}}(u) = \sigma_{\mathcal{A}}(v)}
\end{aligned}
$$

We can define the matrix J where $J_{uv} = 1_{uv \in E} - \frac{1}{2m}\deg(u)\deg(v)$ as in [56]. Then the modularity can be expressed as,

$$
q_{\mathcal{A}}(G) = \frac{1}{2m} \sum_{u,v \in V(G)} J_{uv} 1_{\sigma_{\mathcal{A}}(u) = \sigma_{\mathcal{A}}(v)}.
$$

Thus for the coupling matrix defined above the q-state Potts model with coupling matrix J is related to the modularity of vertex partition $\mathcal{A}_\sigma$ as follows

$$
E_\sigma(G, J) = \exp(-2m q_{\mathcal{A}_\sigma}(G)).
$$

The relationship of modularity to the Potts model has meant that modularity has been studied on lattices, graphs which are of particular interest to the statistical physics community. An extension of the square grid lattice was studied in [27] and a hexagonal lattice structure was considered in [44]. In both of these cases the results are for complete sections. In Chapter 4 we extend these to include any subgraph of a lattice and also graphs which embed 'nicely' into $\mathbb{R}^d$.

1.1.3 Relation to graph theory

In graph theory, much work has been done on minimising the number of edges between parts in a partition of a graph. Suppose we try to find the partition of a graph G into two non-empty parts which minimises the number of lost edges. Often our best option would be to take a vertex v of minimal degree and take as our two parts, $G \backslash \{v\}$ and $\{v\}$. This is technically a bipartition but it's not considered interesting and so we need some restriction on the size of the pieces. One option is to require the number of vertices in the two parts to be equal or 1 apart. The minimum number of edges lost in such a bipartition of a graph is called the bisection width of G [18, 49]. Many results already exist for the bisection width of random regular graphs and we will use some of these later in this document. Another option is to find the minimum number of edges lost in an equipartition into k parts as in [17, 48]. Hence there is a general interest of minimising the total edges between parts given a constraint on the size of the parts. We will see that finding partitions with high modularity fits into this class of problems.

In network applications, among others, it often makes sense to expect parts of different sizes, and modularity allows this flexibility. The method by which the modularity function creates a restriction on the sizes desirable in the partition is via the degree tax (see definition on p14). As the sum of the degrees is a parameter of the graph, the degree tax is a sum of squares of a set of numbers which have a given sum. Thus the degree tax is minimised by taking many parts and, for a fixed number of parts, it is minimised by taking the degree sums of those parts to be as equal as possible. The behaviour of the degree tax gives rise to an interesting optimisation problem of maximising the number of edges within parts without having to set explicit size restrictions for these parts.

Modularity is an example of a judicious partitioning problem. This term refers to partitioning problems in which one is trying to optimise multiple parameters simultaneously. Examples are partitioning two or more different edge sets on the same vertex set [37, 51], creating partitions where each part is incident with many edges [9, 29], dividing the vertices into two equally sized parts such that both have few edges inside [8] and also, for directed graphs dividing the vertices into two equally sized parts so that there are many edges 'going each way' between the two parts [39].

If you want to maximise one quantity it is sometimes enough to construct a random partition, calculate the expected value of your desired quantity. The first moment method then guarantees existence of a partition achieving this bound. Now suppose you want to maximise quantities 'a' and 'b'. You can calculate the expected values of each quantity separately but there is no guarantee of a partition which simultaneously achieves at least the expected values of both quantities, see [10] for further discussion. The two parameters make modularity an interesting function to study theoretically, both constructing partitions that simultaneously give high edge contribution and low degree tax and also the challenge of proving the non-existence of such a vertex partition when showing upper bounds to the maximum modularity of a graph.

1.1.4 Contribution and outline of the thesis.

Given the prominence of modularity in community detection it is an important function to understand mathematically.

We develop new results in the five areas below. The most significant contribution is the last one, an analysis of the evolution of the maximum modularity of Erdős-Rényi random graphs as the edge probability increases.

Isoperimetric constants ∼ Chapter 2
With the exception of the cycle and complete graph for which Brandes et al. showed the precise modularity, all previous results on the modularity are lower bounds. To get a lower bound on modularity it suffices to construct a vertex partition and prove it has the modularity claimed. This thesis provides the first rigorous upper bounds in modularity for some general graph classes and upper bounds derived from graph properties.

We establish techniques in Chapter 2 where we prove upper bounds on modularity as a function of isoperimetric parameters. See in particular Theorem 2.1.1 for an application of the probabilistic method which shows the maximum modularity of a graph is bounded above by a function of its edge expansion.

Modularity of graph classes
Finding the modularity for classes of graphs helps us understand the behaviour of the modularity function.

Trees and graphs with low treewidth ∼ Chapter 3
The modularity of low degree trees was shown to be asymptotically maximal by Bagrow [2] and De Montgolier et al. [16]. In Theorem 3.1.1 we extend this result to cover all graphs where the product of the treewidth and the maximal degree is much less than the number of edges. Any graph where one can delete a small proportion of the edges to leave a forest of sublinear degree is also shown to have high modularity in Lemma 3.2.2.

Lattices and lattice-like networks ∼ Chapter 4
Modularity in lattices and lattice-like networks. In their paper, Guimera et al. [2] determine the modularity of a complete rectangular section of the integer lattice. We extend this result and show that deleting any number of edges in such a lattice achieves this modularity or better asymptotically. More generally we show approximately optimal modularity for networks with certain geometric properties. This includes all lattice configurations previously analysed individually.

Random Graphs
A differentiation between graphs which are truly modular and those which are not can ... only be made if we gain an understanding of the intrinsic modularity of random graphs. – Reichardt and Bornholdt [56].

The maximum modularity of random graphs has been explored in simulations and using heuristic arguments which assume, for example, that optimal partitions must have parts of equal sizes and/or a constant number of parts [27, 55, 56]. In [59] the significance of a partition is explored using subgraph counts.

Random Regular Graphs $\sim$ Chapter 5
We give an upper bound on the modularity of r-regular graphs in terms of the edge expansion of small sets. This leads to results for random r-regular graphs. In particular we show the modularity of a random cubic graph is whp in the interval $(0.66, 0.81)$. Our results give the best thresholds for the statistical significance in large regular networks for $r = 3, \ldots, 12$.

Erdős-Rényi random graphs $\sim$ Chapter 6
We study the maximum modularity of a Erdős-Rényi random graph near criticality. Our main finding is three different phases of modularity dependent on the edge probability. This forms Theorem 6.1.1. For a flavour of the result, consider the random graph with edge probability $p = c/n$ and c constant. Recall that the modularity of any graph is in the range $[0, 1)$, with higher values indicating a better modularity score. For $0 < c \leq 1$ whp the maximum modularity is $1 - o(1)$. For constant $c > 1$, there is a $\varepsilon = \varepsilon(c)$ such that whp the maximum modularity is in the range $(\varepsilon, 1 - \varepsilon)$, with more precise bounds given in Theorem 6.1.4. Lastly for $np \to \infty$ we show that whp the modularity is $o(1)$.

The structure of an optimal partition exhibits interesting behaviour. In Theorem 6.1.5 we prove taking the vertex sets of the connected components is whp the optimal partition for a random graph with edge probabilities small up to a point in the lower window of the phase transition for the giant component. For some larger values of edge probability this partition based on connected components is no longer optimal. Performance of different constructions is investigated in Section 6.2. We prove the maximum modularity to be highly concentrated in Theorem 6.6.1.

1.2 Notation and definitions

Here we define the bulk of the symbols needed for the thesis. Some more specific definitions which are used in only a small section of the thesis are defined when needed, such as treewidth in Chapter 3 and vector geometry notation in Chapter 4. Each symbol and term is also listed in the index with a pointer to where it is defined shown in bold.

Graph Theory

We write $G = (V, E)$ for the graph G with vertex set $V = V(G)$ and edge set $E = E(G)$. All graphs will be simple, loopless and undirected unless otherwise stated. Write $m = |E|$ for the number of edges, sometimes $e(G)$ if we want to emphasise which graph, and $n = |V|$ for the number of vertices. The edge set is a set of two element subsets of the vertices, i.e. $E(G) \subseteq \binom{V(G)}{2}$. The edge (u, v) will be denoted uv, but the order has no meaning. The vertices u and v are referred to as endpoints of the edge uv. If $uv \in E(G)$ we say that u is adjacent to v also that v is adjacent to u and that both vertices u and v are incident with the edge uv. The neighbourhood of v, denoted $\Gamma(v)$ is the set of vertices incident to v. The closed neighbourhood is defined to be $\overline{\Gamma}(v) = \Gamma(v) \cup \{v\}$. The size of the (non-closed) neighbourhood is called the degree of v in G, $\deg_G(v) = \deg(v) = |\Gamma(v)|$, where G is mentioned only if not clear from context. We say vertex with degree 0 is an isolated vertex. The maximal degree of the graph is denoted $\Delta = \Delta(G) = \max_{v\in G} \deg(v)$.

For vertex subsets $A, B \subseteq V(G)$, $E(A)$ is the set of edges with both endpoints in A and $E(A, B)$ is the set of edges with one endpoint in A and one endpoint in B. We write $e(A) = |E(A)|$ and $e(A, B) = |E(A, B)|$, again writing $e_G(A)$ and $e_G(A, B)$ if the graph under consideration is not clear from context. We write $\mathrm{ds}(A)$ for the sum of degrees of the verties in A, i.e. $\mathrm{ds}(A) = \sum_{v\in A} \deg(v)$. Importantly, this degree includes all edges incident to v not just those with both endpoints in A, so $\mathrm{ds}(A) = 2e(A) + e(A, V\backslash A)$. The symmetric difference between sets A and B, denoted $\triangle$ is defined to be $A\triangle B = (A\backslash B)\cup(B\backslash A)$.

We say a graph is connected if for all distinct pairs of vertices u, v there is a path between them. A regular graph is one in which all vertices have the same degree, we call it an r-regular graph if the common degree of all vertices is r. For $r = 3$, we call it a cubic graph. We say the excess of a connected component C is $\ell(C) = e(C) - |C|$. Note if C is a tree then $\ell(C) = -1$. The excess of a graph is the sum of the excesses of its non-tree connected components i.e. $\ell(G) = \sum_{C:\ell(C)\geq 0} \ell(C)$.

Asymptotic and probabilistic notation

We use the standard Landau notation $O(\cdot), o(\cdot)$. When an event holds with probability tending to 1 as $n \to \infty$ we say it holds with high probability which we abbreviate as whp. In our discussion of probabilistic results we will sometimes say the likely maximum modularity of a random graph is x as shorthand for the statement that whp the random graph has maximum modularity of x. Also for functions $a(n), b(n)$ write $a \ll b$ if $a = o(b)$. We write $a \sim b$ if $a = b(1+o(1))$ with the convention that $a \sim 0$ means $a = o(1)$. An 'inequality' version will also be needed. This is less standard so we define it below.

Definition 1.2.1 (nearly greater than, $\succeq$, nearly less than, $\preceq$)**.** *We write* $a \succeq b$ *if* $a > b(1 + o(1))$ *and similarly write* $a \preceq b$ *if* $a < b(1 + o(1))$.

We now have enough notation to sensibly discuss modularity. Other, more specific notation will be introduced when needed. Refer to the index on p156 to be directed to the definitions of the symbols and terms used in the thesis. The rest of this introductory chapter is devoted to surveying and clarifying previous results, proving elementary properties of modularity and establishing some preparatory lemmas for later use.

1.3 Graph classes and modularity

Finding the modularity for various graph classes helps us understand the behaviour of the modularity function. We show in the table on p24 the best known results for the modularity of graph classes. The contributions of previous authors is described in Section 1.3.2. When the result is novel the table provides a pointer to the place in the thesis where it is proved. Some of our new results on graph classes are intricate and entire chapters are devoted to them, e.g. trees and lattices. In Section 1.3.3 we provide the shorter new results.

1.3.1 A Modularity Zoo

We identify three important possible behaviours for the modularity of a graph class.

Define a sequence of graph $\{G_m\}$ where G_m has $m \geq 1$ edges. Then we say that $\{G_m\}$ is *perfectly modular* if $q^*(G_m) \to 1$ as $m \to \infty$, *critcally modular* if $\exists \varepsilon > 0$ such that for each G_m, $\varepsilon < q^*(G_m) < 1 - \varepsilon$ and *non-modular* if $q^*(G_m) \to 0$ as $m \to \infty$.

We also define a probabilistic notion of the three classes. For these we parametrise by the number of vertices. Denote these graph sequences as $\{G_n\}$ where G_n has n vertices. If G_n is a random graph, we say that $\{G_n\}$ is *whp perfectly modular* if, $q^*(G_n) = 1 + o(1)$ whp, i.e. $\exists \{\varepsilon_n\}$ such that $\varepsilon_n \to 0$ and $\mathbb{P}(q^*(G_n) > 1 - \varepsilon_n) \to 1$ as $n \to \infty$. The notions of *whp critically modular* and *whp non-modular* are defined analagously.

The table on p24 displays the results on modularity of various graph classes, sorted into these three categories. The last columns provides a pointer to the place in the thesis where the result is discussed.

1.3.2 Previous work

We make a catalogue of the results of previous authors on the maximum modularity of graphs. This contribution includes results on cycles, complete graphs, trees and a graph termed a 'torus graph' which we define below. The maximum modularity of cycles and complete graphs was asymptotically determined, see Lemmas 1.3.1 and 1.3.2. For the other graphs, only lower bounds on the maximum modularity were obtained.

Perfectly Modular			
Cycle	C_m	$q^*(C_m) = 1 - 2m^{-1/2}(1+o(1))$	Brandes et al. [13], see Lemma 1.3.1, p25.
Tree	$T_m \;:\; \Delta(T_m) = o(n)$	$q^*(T_m) \geq 1 - 2(2\Delta/m)^{1/2}$	Theorem 3.1.1, p62
Tree-like	$G_m \;:\; \Delta(G_m)\mathrm{tw}(G_m) = o(n)$	$q^*(T_m) \geq 1 - 2((t+1)\Delta/m)^{1/2}$	Theorem 3.1.1,p62
Lattice	1-lattice	$q^*(L_m) = 1 - \Theta(m^{-\frac{1}{d+1}})$	Theorem 4.4.1, p87
Lattice	ℓ-lattice: d, ℓ fixed	$q^*(L_m) = 1 - O(m^{-\frac{1}{d+1}})$	Guimerà et al. [27], see Lemma 4.1.1, p73
Sublattice	subgraph of ℓ-lattice	$q^*(L_m) = 1 - O(\sqrt{d}\ell^{\frac{2d}{d+1}} m^{-\frac{1}{d+1}})$	Theorem 4.2.1, p74
Lattice-like	$\exists \alpha : V(G_m) \to \mathbb{R}^d$ such that		
	$\forall x \neq y \in V : \\|\alpha(x) - \alpha(y)\\| \geq 1$ $\forall vw \in E : \\|\alpha(v) - \alpha(w)\\| \leq \ell$	$q^*(L_m) = 1 - O(d\ell^{\frac{2d}{d+1}} m^{-\frac{1}{d+1}})$	Theorem 4.3.1, p74
(whp) Random Planar	G_n	(whp) $q^*(G_n) = 1 - O(\log n/\sqrt{n})$	Corollary 3.1.3, p62
(whp) Erdős-Rényi	$G_n \sim \mathcal{G}(n,p)$		
	for $n^2 p \to \infty$ & $np \leq 1 + o(1)$	(whp) $q^*(G_n) = 1 + o(1)$	Theorem 6.1.1, p96
Critcally Modular			
(whp) Erdős-Rényi	$G_n \sim \mathcal{G}(n,p)$ for constant $c > 1$		
	and $np = c + o(1)$	see Theorem	Theorem 6.1.1, p96
(whp) Random Cubic	G_n	(whp) $0.66 < q^*(G_n) < 0.81$	Theorem 5.2.1, p94
(whp) Random Regular	random r-regular graph		
	for $r = 4, \ldots, 12$	see Theorem	Theorem 5.2.1, p94
Non-Modular			
Complete Graph	K_n	$q^*(K_n) = 0$	Brandes et al. [13], see Lemma 1.3.2, p26.
Complete Bipartite	K_{n_1,n_2}	$q^*(K_{n_1,n_2}) = 0$	Theorem 1.3.5, p29
Balanced Turán	G_n	$q^*(G_n) = 0$	Theorem 1.3.4, p27
(whp) Erdős-Rényi	$G_n \sim \mathcal{G}(n,p)$ for $np \to \infty$	(whp) $q^*(G_n) = o(1)$	Theorem 6.1.1, p96

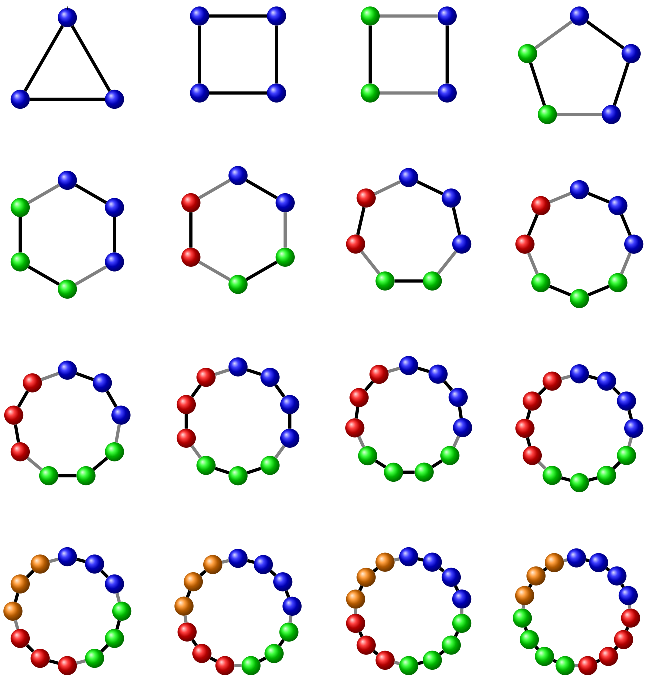


Figure 1.2: Illustration of some small cycles and their optimal partition(s) (up to rotation).

Cycles

The maximum modularity of cycles is proven in Theorem 6.7 of [13] which we repeat as Lemma 1.3.1 below.

Lemma 1.3.1 (Brandes et al. [13]). *Let C_n be a cycle on n vertices. Then*

$$q^*(C_n) = 1 - 2n^{-1/2}(1 + o(1)).$$

Brandes et al. also show that any optimal partition of a cycle on n vertices will be formed of connected pieces of the cycle of length $\sqrt{n}(1 + o(1))$ (a more exact expression is given in their paper). See Figure 1.2 for the optimal partitions of some small cycles.

Complete graphs

The same paper which contains the cycle result proves that the maximum modularity of a complete graph is 0, see Theorem 6.3 of [13].

Lemma 1.3.2 (Brandes et al [13])**.** *Let K_n be the complete graph on n vertices. Then*

$$q^*(K_n) = 0.$$

The cycle and complete graphs were the only graphs for which the maximum modularity was previously known, for all other graphs only lower bounds were established.

Trees

The modularity of trees and tree-like networks was first investigated by Bagrow in a paper whose title we borrow for a chapter heading [2]. They looked at the k-ary tree, i.e. the tree in which each node has k children, for g generations. For at least two generations of fertile nodes they show the modularity of this tree approaches 1 as the number of generations is fixed and k increases. They also show high modularity in simulations of Galton-Watson trees.

A more general class of trees was considered in [16]. In this paper De Montgolfier et al. show that any tree with maximum degree $o(n^{1/5})$ has modularity approaching 1 as $n \to \infty$. We extend this result to any tree with maximum degree $o(n)$, see Theorem 3.1.1.

Torus graphs and lattices

To describe the last graph class we need some new notation. Two sets of authors have results on what they term torus graphs and lattice graphs respectively which can both be defined as products of paths and cycles. Denote $[\ell] = \{1, \dots, \ell\}$.

Definition 1.3.1 (Path P_n^ℓ, Cycle C_n^ℓ)**.** *Define P_n^ℓ to be the graph with vertex set $P = \{v_i\}_{i \in [n]}$ and edge set $E = \{v_i v_j : \ i - j \in [\ell]\}$ and define C_n^ℓ to be the graph with the same vertex set and edge set $E = \{v_i v_j : \ i - j \mod n \in [\ell]\}$.*

Note that for $\ell = 1$ these are the usual path and cycle i.e. $P_n = P_n^1$ and $C_n = C_n^1$.

Definition 1.3.2 (Cartesian graph product)**.** *Define $\prod_{i=1}^d G_i$ to be the graph with vertex set $V = \prod_{i=1}^d V(G_i)$ and edge set $E = \{\underline{uv} : \ \exists j \text{ such that } u_j v_j \in E(G_j) \text{ and } u_i = v_i \ \ \forall i \neq j\}$.*

An illustration of $P_4^2 \times P_6^2$ and $P_4^3 \times P_6^3$ can be found in Figure 4.1 on p72. Note the cartesian product is sometimes called the box product and denoted $\Box$, which helps distinguish it from other graph products and also acts as visual mnemonic: the cartesian product of K_2 with itself is the cycle C_4. However, we will use only this notion of graph product and so denote it as a simple product '×'.

Graphs formed as the cartesian product of cycles C_k^ℓ were studied by De Montgolfier et al. for $\ell = 1$ and by Guimerà [27] for $\ell \geq 1$. Chapter 4 is dedicated to studying the maximum modularity of lattice graphs and we describe the results of Guimerá in detail there, see p73.

Lemma 1.3.3 (De Montgolfier et al. [16])**.** *Let $\underline{k} \in \mathbb{N}^d$, $n = \prod_i k_i$ and $G = \prod_{i=1}^d C_{k_i}$. Then for constant d,*

$$q^*(G) \geq 1 - O(n^{-\frac{1}{2d}}).$$

We improve on this lemma in Chapter 4. Notice that for constant d in the graph defined above the number of edges and number of vertices have the same order of magnitude, i.e. $m = \Theta(n)$. Hence, assuming the same conditions as Lemma 1.3.3, our Theorem 4.2.1 implies directly that $q^*(G) \geq 1 - O(n^{-\frac{1}{d+1}})$. For the special case that the k_i's are all equal we can show this is the right order of magnitude. More precisely, for equal k_i, we determine the modularity of $G = \prod_{i=1}^d C_{k_i}$ to be $q^*(G) = 1 - \Theta(n^{-\frac{1}{d+1}})$ in Theorem 4.4.1.

1.3.3 Elementary new results

This thesis vastly extends set of graph classes for which the modularity is known. Some of these results are intricate, for example on the modularity of trees, lattices and random graphs and so have dedicated chapters later in the thesis. This section has results which are new but have short proofs, so we present them here. We first prove, Theorem 1.3.4, that the maximum modularity of complete balanced multipartite graphs is 0. We also show maximum modularity of 0 for any (not necessarily balanced) complete bipartite graph in Theorem 1.3.5. However we also show in Lemmas 1.3.6 and 1.3.7 that either adding or removing an edge from such a graph can give strictly positive maximum modularity.

Balanced Turán graphs have modularity zero

A Turán graph $T_d(n)$ has d disjoint independent sets with all edges present between distinct sets and the sizes of the independent sets are different by at most 1. Thus it is a special case of a complete d-partite graph, for example $T_2(n)$ is a complete bipartite graph with two equal or nearly equal sized parts. The next theorem concerns balanced Turán graphs where we require the disjoint independent sets to be exactly the same size.

Theorem 1.3.4. *Let $T_d(n)$ be the balanced Turán graph with d disjoint independent sets of size c and $n = cd$ vertices. Then $q^*(T_d(n)) = 0$.*

Proof. Fix a vertex partition $\mathcal{A} = \{A_1, \dots, A_k\}$. Denote by $V_1, \dots, V_d$ the independent sets of $T_d(n)$ and let $x_{i,u} = |A_i \cap V_u| - \frac{c}{k}$. We can write the edge contribution and degree tax in terms of these variables which measure the distance from an equipartition. Note $\sum_{u=1}^{d} \sum_{i=1}^{k} x_{u,i} = 0$, the number of edges is $m = c^2 \binom{d}{2}$ and the graph is regular with degree $c(d-1)$.

$$
\begin{aligned}
mq_{\mathcal{A}}^{E}(T_d(n)) &= \frac{1}{2}\sum_{i=1}^{k}\sum_{u\neq v}\left(\frac{c}{k}+x_{u,i}\right)\left(\frac{c}{k}+x_{v,i}\right) \\
&= \frac{m}{k} + \frac{1}{2}\sum_{i=1}^{k}\sum_{u\neq v} x_{u,i}x_{v,i}. \qquad (1.1)\\
n^2 q_{\mathcal{A}}^{D}(T_d(n)) &= \sum_{i=1}^{k}\left(\frac{n}{k}+\sum_{u=1}^{d} x_{u,i}\right)^2 \\
&= \frac{n^2}{k} + \frac{2n}{k}\sum_{i=1}^{k}\sum_{u=1}^{d} x_{u,i} + \sum_{i=1}^{k}\left(\sum_{u=1}^{d} x_{u,i}\right)^2 \\
&= \frac{n^2}{k} + \sum_{i=1}^{k}\sum_{u\neq v} x_{u,i}x_{v,i} + \sum_{i=1}^{k}\sum_{u=1}^{d} x_{u,i}^2. \qquad (1.2)
\end{aligned}
$$

Now write the modularity of $q_{\mathcal{A}}(T_d(n))$ and many terms in (1.1) and (1.2) cancel.

$$
\begin{aligned}
q_{\mathcal{A}}(T_d(n)) &= \frac{1}{d^2(d-1)c^2}\sum_{i=1}^{k}\left(\sum_{u\neq v} x_{u,i}x_{v,i} - (d-1)\sum_{u=1}^{d} x_{u,i}^2\right) \\
&= \frac{1}{d^2(d-1)c^2}\sum_{i=1}^{k}\left(\left(\sum_{u=1}^{d} x_{u,i}\right)\left(\sum_{v=1}^{d} x_{v,i}\right) - d\sum_{u=1}^{d} x_{u,i}^2\right) \qquad (1.3)\\
&\leq 0. \qquad (1.4)
\end{aligned}
$$

By Cauchy-Schwarz, for each i the expression in the sum in (1.3) will be at most 0 which implies the last inequality. □

Notice we assumed that the parts of our complete multipartite graphs were the same size. For the special case of two parts we can remove this condition as we now show in Theorem 1.3.5. It is unknown whether the balanced condition on the part sizes in Theorem 1.3.4 is necessary and this would be interesting to investigate.

Theorem 1.3.5. *Suppose we have a complete bipartite graph G on vertex sets U, V and let $\mathcal{A} = \{A_1, \ldots, A_k\}$ be any partition. Then $q_{\mathcal{A}}(G) \leq 0$.*

Proof. Write $U_i = A_i \cap U$, $V_i = A_i \cap V$, $u_i = |U_i|$ and $v_i = |V_i|$ as shown in Figure 1.3.

Observe that the number of edges within part A_i is $u_i v_i$ and so $\sum_i e(A_i) = \sum_i u_i v_i$. The total number of edges in G is $m = |U||V|$ and hence the edge contribution is

$$q^E_{\mathcal{A}}(G) = \frac{1}{|U||V|} \sum_i u_i v_i.$$

To calculate the degree tax note the degree of any vertex in U is $|V|$ (and similarly a vertex in V has degree $|U|$) which implies $\mathrm{ds}(A_i) = u_i|V| + v_i|U|$. Therefore the degree tax is

$$q^D_{\mathcal{A}}(G) = \frac{1}{4|U|^2|V|^2} \sum_i \Big(u_i|V| + v_i|U|\Big)^2.$$

Combining this with the expression for the edge contribution we can write the modularity of $\mathcal{A}$ and some terms cancel

$$\begin{aligned} q_{\mathcal{A}}(G) &= \frac{1}{4|U|^2|V|^2} \sum_i 4u_i v_i |U||V| - \Big(u_i^2|V|^2 + 2u_i v_i |U||V| + v_i^2 |U|^2\Big) \\ &= \frac{1}{4|U|^2|V|^2} \sum_i 2u_i v_i |U||V| - u_i^2|V|^2 - v_i^2|U|^2. \end{aligned} \tag{1.5}$$

Notice by the Cauchy-Schwarz inequality $\sum_i u_i v_i \leq \sqrt{(\sum_i u_i^2)(\sum_i v_i^2)}$. This inequality and line (1.5) then give the result

$$\begin{aligned} q_{\mathcal{A}}(G) &\leq \frac{1}{4|U|^2|V|^2} \Big(2\Big(\sum_i u_i^2\Big)^{\frac{1}{2}}\Big(\sum_i v_i^2\Big)^{\frac{1}{2}}|U||V| - \Big(\sum_i u_i^2\Big)|V|^2 - \Big(\sum_i v_i^2\Big)|U|^2\Big) \\ &= \frac{-1}{4|U|^2|V|^2}\Big(\Big(\sum_i u_i^2\Big)^{\frac{1}{2}}|V| - \Big(\sum_i v_i^2\Big)^{\frac{1}{2}}|U|\Big)^2 \\ &\leq 0. \end{aligned}$$

□

By the previous theorem a complete bipartite graph has modularity 0. We now show that the graphs $K_{2a,2b} - e$ and $K_{2a,2b} + e$ both have strictly positive modularity. These two constructions are used to show that the maximum modularity is not monotone under taking subgraphs in Example 1.4.4.

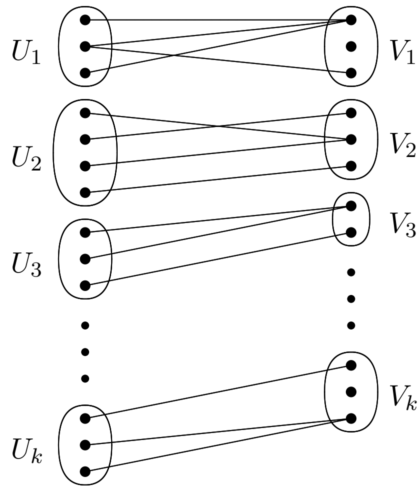


Figure 1.3: Bipartite graph partitioned into k clusters.

Complete bipartite graph minus an edge

In the following lemma we show that the graph constructed by taking a complete bipartite graph on partite vertex sets of sizes $2a$ and $2b$ and then removing any one edge has strictly positive modularity.

Lemma 1.3.6. *Let a and b be positive integers and $K_{2a,2b} - e$ be a graph constructed by removing any edge from the complete bipartite graph $K_{2a,2b}$. Then*

$$q^*(K_{2a,2b} - e) > 0$$

Proof. Let G be the graph $K_{2a,2b} - e$. Label the vertices in the two parts of G by $\{u_1, \ldots, u_{2a}, v_1, \ldots, v_{2b}\}$ such that $u_i v_j$ is an edge if and only if $i + j > 2$. Then define the vertex partition $\mathcal{A} = \{A_1, A_2\}$ by $A_1 = \{u_1, \ldots, u_a, v_{b+1}, \ldots, v_{2b}\}$ and $A_2 = \{u_{a+1}, \ldots, u_{2a}, v_1, \ldots, v_b\}$. We will show $q_{\mathcal{A}}(G) > 0$. The degree tax is $q_{\mathcal{A}}^D(G) = \frac{1}{2}$. Hence it will be sufficient to show $q_{\mathcal{A}}^E(G) > \frac{1}{2}$. We do this by calculating the edge contribution precisely, write $m = e(G)$,

$$q_{\mathcal{A}}^E(G) = \frac{1}{m}\Big(e(A_1) + e(A_2)\Big) = \frac{2ab}{4ab - 1} > \frac{1}{2}.$$

□

Complete bipartite graph plus an edge

Similar to above, we now show that the graph constructed by taking a complete bipartite graph on partite vertex sets both of even size at least four and then adding any one edge also has strictly positive modularity.

Lemma 1.3.7. *Let $a, b \geq 2$ be integers and $K_{2a,2b}+e$ be a graph constructed by adding any edge to the complete bipartite graph $K_{2a,2b}$. Then*

$$q^*(K_{2a,2b} + e) > 0.$$

Proof. Let G be the graph $K_{2a,2b} + e$. Label the vertices in the two parts of G by $\{u_1, \ldots, u_{2a}, v_1, \ldots, v_{2b}\}$ such that $u_i v_j$ is an edge for all i, j and also $u_1 u_2$ is an edge. Then define the vertex partition $\mathcal{A} = \{A_1, A_2\}$ by $A_1 = \{u_1, \ldots, u_a, v_1, \ldots, v_b\}$ and $A_2 = \{u_{a+1}, \ldots, u_{2a}, v_{b+1}, \ldots, v_{2b}\}$. Note that because $n \geq 2$ the extra edge $u_1 u_2$ will be in the part A_1. We will show $q_{\mathcal{A}}(G) > 0$ by calculating both the edge contribution and degree tax explicitly; write m for $e(G)$,

$$\begin{aligned}
q^E_{\mathcal{A}}(G) &= \frac{1}{m}\Big(e(A_1) + e(A_2)\Big) = \frac{2ab+1}{4ab+1} = \frac{1}{2} + \frac{\frac{1}{2}}{4ab+1}. \\
q^D_{\mathcal{A}}(G) &= \frac{1}{m}\Big((2e(A_1) + e(A_1, A_2))^2 + (2e(A_2) + e(A_1, A_2))^2\Big) \\
&= \frac{(4ab+2)^2 + (4ab)^2}{(8ab+2)^2} = \frac{8a^2b^2 + 4ab + 1}{(4ab+1)^2} = \frac{1}{2} + \frac{\frac{1}{2}}{(4ab+1)^2}.
\end{aligned}$$

Thus $q^E_{\mathcal{A}}(G) - q^D_{\mathcal{A}}(G) > 0$ and we are done. □

1.4 Graph operations and modularity, monotonicity?

In this section we present several different ways to perturb our graph G and study the effect on the resulting modularity.

1.4.1 Detachments

Imprecisely speaking we get a graph H as a detachment of G by dividing vertices so that each edge incidident with the original vertex is incident with exactly one of these divided vertices in H. This operation can only cause the modularity to increase or stay the same. We use the definition from [21].

Definition 1.4.1. *Let G be a graph with vertex set $V(G) = v_1, \dots, v_n$ vertices. We say a graph H is a detachment of G if there is a vertex partition of H, $\mathcal{I} = \{I_1, \dots, I_n\}$ such that each I_i is an independent set and*

$$e_H(I_i, I_j) = \begin{cases} 1 & \text{if } v_i v_j \in E(G) \\ 0 & \text{otherwise} \end{cases}.$$

We show that performing this detachment operation can only improve (or at least equal) the modularity.

Lemma 1.4.1. *Let H be a detachment of G. Then $q^*(H) \geq q^*(G)$.*

Proof. Let G be a graph on m edges with vertex set $\{v_1, \dots, v_n\}$. Suppose H is a detachment of G and fix a vertex partition $\mathcal{I}$ of H satisfying the conditions in the definition of detachment. By definition of detachment H must also have exactly m edges.

Let $\mathcal{A} = \{A_1, \dots, A_k\}$ be an optimal partition of G and construct a vertex partition $\mathcal{A}'$ of H by

$$A'_j = \bigcup_{i \,:\, v_i \in A_j} I_i.$$

For each j, I claim that $e_H(A'_j) = e_G(A_j)$. Every $I_i \in V(H)$ is an independent set in H so the number of edges in A'_j in H is the number of edges between each set I_i which is a subset of A'_j, i.e. $e_H(A'_j) = \sum_{I_i \neq I_\iota \subset A'_j} e(I_i, I_\iota) = \sum_{v_i \neq v_\iota \in A_j} e(I_i, I_\iota) = e_G(A_j)$, which confirms the claim. As $e(H) = e(G)$ this implies the edge contributions will be the same, $q^E_{\mathcal{A}'}(H) = q^E_{\mathcal{A}}(G)$. □

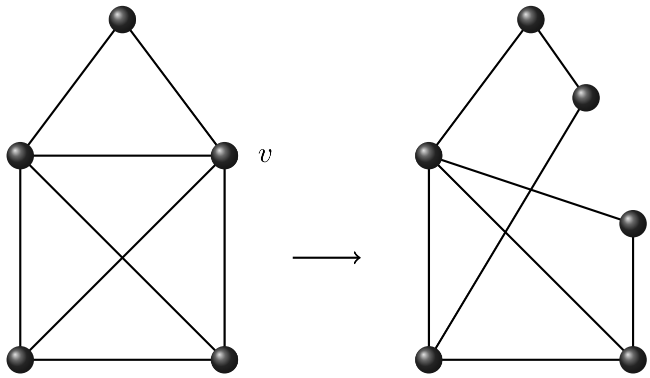


Figure 1.4: An illustration of a detachment operation. In this example the vertex v is replaced by two vertices each of which is joined to two neighbours of v in the original graph. Notice the neighborhoods of the two vertices are disjoint but their union is the original neighborhood of v.

Corollary 1.4.2. *Let G be a graph with m edges. Then $q^*(G) \geq 1 - 1/m$ with equality if and only if the m edges in G are disjoint.*

Proof. Consider the following operation. If any vertex v in graph G^i has degree $d > 1$ then create a new graph G^{i+1} by replaying v with an indpendent set of vertices such that each is adjacent to exactly one of the neighbours of v in G^i. As G^{i+1} is a detachment of G^i, $q^*(G^{i+1}) \geq q^*(G^i)$.

Let the initial graph be $G = G^1$ and create a sequence $G^1, G^2, \ldots$ as above. Each time the operation is performed, the number of vertices with degree more than 1 is stricly decreased, so this process must stop. Hence we have some G^j where $q^*(G^j) \geq q^*(G)$ and the degree of every vertex in G^j is either 0 or 1. Denote by V_0 the set of isolated vertices in G^j and Lemma 1.4.8 implies $q^*(G^j \backslash V_0) = q^*(G^j)$. It will suffice to show that $q^*(G^j \backslash V_0) = 1 - 1/m$.

The modularity of $G^j \backslash V_0$ is easy to calculate. Each vertex in $G^j \backslash V_0$ has degree 1 so the graph consists of m disjoint edges on $2m$ vertices. By Karamata's inequality, Lemma 1.6.9, the optimal partition is to put each of the m disjoint edges into a distinct part. As each edge is within a part, the edge contribution is 1. The degree sum of each part is 4, and so the degree tax is $m \times 4/(4m^2) = 1/m$. Hence $q^*(G^j \backslash V_0) = 1 - 1/m$ as required. □

1.4.2 Blowups

The graph operation, blowups, create larger graphs from smaller graphs in which the larger graphs retain some of the same features of the original graphs. They are used extensively in problems concerning subgraph counts. The exact definition is given below. We show in Theorem 1.4.3 that modularity is monotone non-decreasing under this operation.

Definition 1.4.2 (blowups)**.** *For a graph G and $a \in \mathbb{N}$ define the b-blowup of G to be the graph obtained by replacing each vertex $v_i \in G$ with an independent set I_i of b vertices and by replacing each edge $v_iv_j \in G$ with a complete bipartite graph connecting the empty sets I_i and I_j. We say that H is a blowup of G if there is some b such that H is the b-blowup of G.*

Theorem 1.4.3. *Let G be a graph and H a blowup of G. Then $q^*(H) \geq q^*(G)$.*

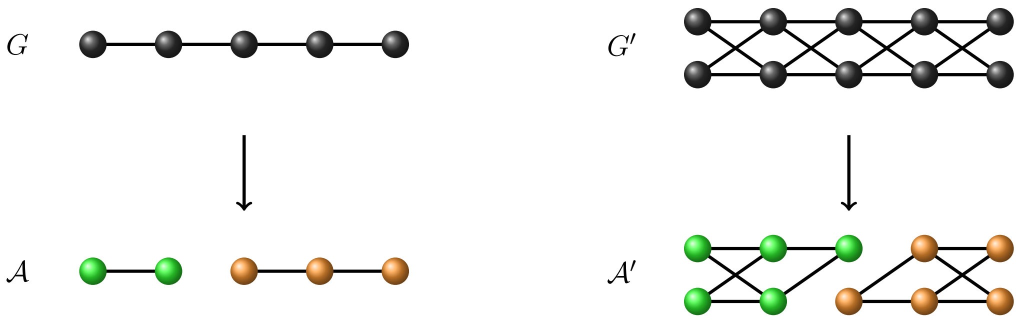
Proof. Let G be a graph on m edges and suppose H is an b-blowup of G. We write $\{v_1, \ldots, v_n\}$ for the vertices of G and I_i for the independent set in H which replaced vertex $v_i \in V(G)$.

Let $\mathcal{A} = \{A_1, \ldots, A_k\}$ be an optimal partition of G. We will construct a vertex partition $\mathcal{A}'$ of H such that $q_{\mathcal{A}'}(H) = q_{\mathcal{A}}(G)$. We define $\mathcal{A}' = \{A'_1, \ldots, A'_k\}$ where

$$A'_j = \bigcup_{i\,:\,v_i \in A_j} I_i.$$

We replaced each edge in G by a complete bipartite graph of b^2 edges in H, and if an edge was within part A_j in G then all edges of the complete bipartite graph which replaced it are within A'_j in H. Thus $e(H) = b^2 m$ and $e_H(A'_j) = b^2 e_G(A_j)$ which together implies $q^E_{\mathcal{A}'}(H) = q^E_{\mathcal{A}}(G)$. Now consider the degree tax. Each vertex in v_i in G is replaced by b vertices, each of which are incident to a factor of b times as many vertices in H as v_i was incident to in G. Hence $\mathrm{ds}_H(I_i) = b^2 \deg_G(v_i)$ and $\mathrm{ds}_H(A'_i) = b^2 \mathrm{ds}_G(A_i)$. As the number of edges also increased by the same factor, b^2, the degree taxes are equal: $q^D_{\mathcal{A}'}(H) = q^D_{\mathcal{A}}(G)$, which proves our result. □

Note there is sometimes a strict increase in the modularity of a blowup: take the path on five vertices P_5 and its 2-blowup depicted in Figure 1.5.



$q_{\mathcal{A}}(G) = \frac{3}{4} - \frac{3^2+5^2}{8^2} = \frac{1}{2} - \frac{1}{32}$ $\qquad$ $q_{\mathcal{A}'}(G') = \frac{12}{16} - \frac{8^2+8^2}{16^2} = \frac{1}{2}$

Figure 1.5: A path on five vertices, G, and its blowup G', each shown with an optimal vertex partition. Observe $q^*(G') > q^*(G)$.

1.4.3 Adding or removing edges

Is the maximum modularity of a graph a monotone function over taking subgraphs? In a word no. Example 1.4.4 provides a counterexample. However, if we perturb the edge set only slightly then the change in modularity is also small. This is proven in Theorem 1.4.6.

Example 1.4.4. *We construct graphs G_1, G_2, G_3, G_4 all on the same vertex set with $E(G_1) \subsetneq E(G_2) \subsetneq E(G_3) \subsetneq E(G_4)$ such that $q^*(G_2) = q^*(G_4) = 0$ and $q^*(G_1), q^*(G_3) > 0$. Take $G_1 = K_{4,4} - e$, $G_2 = K_{4,4}$, $G_3 = K_{4,4} + e$ and $G_4 = K_8 - \mathcal{PM}$ where $\mathcal{PM}$ is a perfect matching. Refer to Figure 1.6 for a diagram showing the construction.*

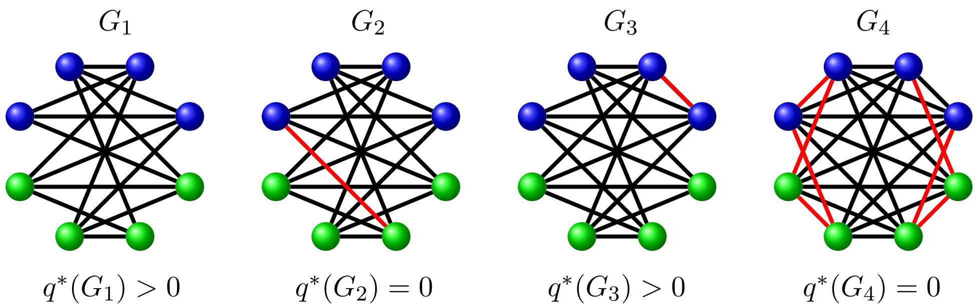


Figure 1.6: The construction in Example 1.4.4 is depicted. Optimal partitions are shown in blue/green. The red edges indicate those edges not contained in the previous graph.

If we fix a graph G with edge set E and a vertex partition $\mathcal{A}$ then we can delete $\alpha|E|$ edges inside parts of $\mathcal{A}$ and $\beta|E|$ edges outside parts of $\mathcal{A}$ without much change in the modularity provided α and β are small.

Lemma 1.4.5. *Fix $\alpha, \beta \geq 0$ such that $0 < \alpha + \beta \leq 1/2$. Let $G = (V, E)$ be a graph and $\mathcal{A}$ a vertex partition of G. Let $E_1, E_2 \subset E$ be such that edges in E_1 lie within parts of $\mathcal{A}$, edges in E_2 lie between parts of $\mathcal{A}$, $|E_1| \leq \alpha|E|$ and $|E_2| \leq \beta|E|$. Define $E' = E \backslash (E_1 \cup E_2)$ and $G' = (V, E')$. Then*

$$-3\alpha - 4\beta < q_{\mathcal{A}}(G) - q_{\mathcal{A}}(G') < 3\alpha + 2\beta.$$

Proof. It suffices to assume $|E_1| = \alpha|E|$ and $|E_2| = \beta|E|$. We first analyse the difference in edge contribution between G and G' where quite crude bounds suffice. In one direction,

$$q^E_{\mathcal{A}}(G) = \frac{1}{|E|}\sum_{A\in\mathcal{A}} e_G(A) \leq \frac{1}{|E|}\left(\alpha|E| + \sum_{A\in\mathcal{A}} e_{G'}(A)\right) \leq \alpha + \frac{1}{|E'|}\sum_{A\in\mathcal{A}} e_{G'}(A) = q^E_{\mathcal{A}}(G') + \alpha,$$

and for the other direction, note $\alpha + \beta < 1/2$ implies $|E| < (1 + 2\alpha + 2\beta)|E'|$,

$$q^E_{\mathcal{A}}(G') = \frac{1}{|E'|}\sum_{A\in\mathcal{A}} e_{G'}(A) < \frac{1}{|E|}(1 + 2\alpha + 2\beta)\left(\sum_{A\in\mathcal{A}} e_G(A) - \alpha|E|\right) \leq q^E_{\mathcal{A}}(G) + \alpha + 2\beta.$$

Now for the degree tax. Observe that $|E|^{-1} \geq |E'|^{-1}(1 - \alpha - \beta)$ and so we can bound the possible increase in degree tax from G to G' by

$$q^D_{\mathcal{A}}(G) = \frac{1}{4|E|^2}\sum_{A\in\mathcal{A}} \mathrm{ds}_G(A)^2 \geq \frac{1}{4|E'|^2}(1 - \alpha - \beta)^2 \sum_{A\in\mathcal{A}} \mathrm{ds}_{G'}(A)^2 > q^D_{\mathcal{A}}(G') - 2\alpha - 2\beta. \quad (1.6)$$

To bound the possible decrease in degree tax from G to G' takes a little work. Define α_i and β_i by $\alpha_i|E| = |E_1 \cap E(A_i)|$ and $\beta_i = |E_2 \cap E(A_i, V\backslash A_i)|$. Note $\sum_i \alpha_i = \alpha$ and $\sum_i \beta_i = 2\beta$. This allows us to relate the degree sums of any part A_i in G and G',

$$\mathrm{ds}_{G'}(A_i) = \mathrm{ds}_G(A_i) - (2\alpha_i + \beta_i)|E|.$$

Thus,

$$\sum_i \mathrm{ds}_{G'}(A_i)^2 \geq \sum_i \mathrm{ds}_G(A_i)^2 - 2|E|\sum_i \mathrm{ds}_G(A_i)(2\alpha_i + \beta_i).$$

For $x_i, y_i \geq 0$, clearly $\sum_i x_i y_i \leq (\sum_i x_i)(\sum_i y_i)$. Hence, recalling $\sum_i \mathrm{ds}_G(A_i) = 2|E|$ and $\sum_i 2\alpha_i + \beta_i = 2(\alpha + \beta)$,

$$\sum_i \mathrm{ds}_{G'}(A_i)^2 \geq \sum_i \mathrm{ds}_G(A_i)^2 - 8|E|^2(\alpha + \beta).$$

This directly implies our last inequality, bounding the possible decrease in degree tax from G to G',

$$q^D_{\mathcal{A}}(G') \geq q^D_{\mathcal{A}}(G) - 2(\alpha + \beta), \quad (1.7)$$

and we are done. □

The precise upper bound of the previous lemma will be needed to prove that whp the maximum modularity of an Erdős-Rényi random graph is $o(1)$ when $np \to \infty$. This result is Lemma 6.4.5, which constitutes a part of our main result of Chapter 6, Theorem 6.1.1, showing the three phases of likely maximum modularity in Erdős-Renyi random graphs.

Lemma 1.4.5 also implies a general bound on the difference in maximum modularity possible after a small perturbation of the edge set.

Theorem 1.4.6. *Fix $0 < \varepsilon < 1$. Let $G = (V, E)$ be a graph. Let $E' \subseteq \binom{V}{2}$ be such that $|E \triangle E'| < \varepsilon|E|/5$ and set $G' = (V, E')$. Then $|q^*(G) - q^*(G')| < \varepsilon$.*

Proof. We define an intermediate graph. Let $E_0 = E \cap E'$ and set $G_0 = (V, E_0)$. Then notice we can perturb G to G_0 by only deleting edges and G_0 to G' by only adding edges. The proof follows by four applications of Lemma 1.4.5.

Define δ, δ' such that $|E \backslash E_0| = \delta|E|$ and $|E' \backslash E_0| = \delta'|E'|$. Let $\mathcal{A}$ be an optimal partition of G, by Lemma 1.4.5 applied to $\mathcal{A}, G$ and G_0,

$$q^*(G) - q_{\mathcal{A}}(G_0) < 3\delta,$$

and since $q_{\mathcal{A}}(G_0) \leq q^*(G_0)$,

$$q^*(G) - q^*(G_0) < 3\delta.$$

Now let $\mathcal{B}$ be an optimal partition of G_0 and Lemma 1.4.5 applied to $\mathcal{B}, G$ and G_0 implies

$$q_{\mathcal{B}}(G) - q^*(G_0) > -4\delta$$

and hence $q^*(G) - q^*(G_0) > -4\delta$. Thus far we have deduced

$$-4\delta < q^*(G) - q^*(G_0) < 3\delta.$$

Similarly, after two applications of Lemma 1.4.5, we bound the difference between the maximum modularities of G' and G_0,

$$-4\delta' < q^*(G') - q^*(G_0) < 3\delta'.$$

Therefore

$$-4\delta - 3\delta' < q^*(G) - q^*(G') < 3\delta + 4\delta'. \tag{1.8}$$

We are almost done. Define δ'' by $\delta''|E| = |E' \backslash E_0|$ and then $|E \triangle E'| = (\delta + \delta'')|E|$. Hence, by assumption $\delta + \delta'' < \epsilon/5$. Now note that $\delta' = \delta''|E'|/|E| < (1 + \epsilon/5)\delta''$. One can then re-arrange (1.8),

$$-4\delta - 3\delta''(1 + \epsilon/5) < q^*(G) - q^*(G') < 3\delta + 4\delta''(1 + \epsilon/5).$$

This finishes the proof: as $0 < \epsilon < 1$ and $\delta + \delta'' < \epsilon/5$, both the upper and lower bounds are less than ϵ. □

In the proof there is some awkwardness because δ' is defined in terms of $|E'|$ but the bound for the symmetric difference in the edge sets is bounded in terms of $|E|$ only. This meant we needed $\epsilon/5$ instead of $\epsilon/4$ control on the symmetric difference. If we instead assumed that $|E \triangle E'| < \frac{\epsilon}{4} \max\{|E|, |E'|\}$ then the result would still hold.

The following technical lemma shows that when changing the edges incident with a particular vertex, the change in the modularity can be bounded above by a function of the degree of this vertex in the graph. It will later help us prove that the maximum modularity of an Erdős-Renyi random graph is concentrated in Theorem 6.6.1 on p142.

Lemma 1.4.7. *Fix a partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ on vertex subset V and fix $v \in V$. Let $G = (V, E)$, $G' = (V, E')$ where the edge sets E, E' differ only in edges incident with v. Write $d = \max\{\deg_G(v), \deg_{G'}(v)\}$. Then if $d \leq |E|/3$,*

$$|q^D_{\mathcal{A}}(G) - q^D_{\mathcal{A}}(G')| \leq \frac{5d}{|E|}.$$

Proof. We define an intermediate graph. As in the proof of Theorem 1.4.6, let $E_0 = E \cap E'$ which is non-empty by assumption, and set $G_0 = (V, E_0)$. Note we can obtain G_0 from G by only deleting edges incident to v and so $|E \backslash E_0| \leq d \leq |E|/3$ so $E_0 \neq \varnothing$. Hence we can apply inequalities (1.6) and (1.7) from the proof of Lemma 1.4.5 to $\mathcal{A}, G$ and G_0 to obtain

$$\frac{-2d}{|E|} \leq q_{\mathcal{A}}(G) - q_{\mathcal{A}}(G_0) \leq \frac{2d}{|E|}.$$

Similarly, applying (1.6) and (1.7) to $\mathcal{A}, G'$ and G_0,

$$\frac{-2d}{|E'|} \leq q_{\mathcal{A}}(G') - q_{\mathcal{A}}(G_0) \leq \frac{2d}{|E'|},$$

and therefore

$$|q_{\mathcal{A}}(G) - q_{\mathcal{A}}(G')| \leq 2d \left(\frac{1}{|E|} + \frac{1}{|E'|} \right). \tag{1.9}$$

Now we are almost done. To finish note $|E'| \geq |E| - d$ and hence because $d \leq |E|/3$, we get $|E'|^{-1} \leq 3|E|^{-1}/2$ and substitute this into (1.9). □

1.4.4 Adding or removing isolated vertices

We can add/remove isolated vertices to/from any graph G and the maximum modularity will not change. As first observed in Corollary 1 of [12] 'isolated vertices have no impact on modularity'. This is made precise below.

Lemma 1.4.8 (Brandes et al. [12])**.** *Let G be a graph with $m \geq 1$ edges and v an isolated vertex. Let $\mathcal{A} = \{A_1, \ldots, A_k\}$ be a partition of $V(G)\backslash\{v\}$. For each $A_j \in \mathcal{A}$ define*

$$\mathcal{A}_j = \{A_1, \ldots, A_j \cup \{v\}, \ldots, A_k\} \text{ and define } \mathcal{A}_0 = \{\{v\}, A_1, \ldots, A_k\}.$$

Then for $j = 0, 1, \ldots, k$,

$$q_{\mathcal{A}_j}(G) = q_{\mathcal{A}}(G\backslash\{v\}).$$

To see why this is true, notice the formula for modularity of a partition $\mathcal{A}$ is a function of only the number of edges and degree sums in the parts of $\mathcal{A}$ and hence it is blind to isolated vertices. In particular, the modularity is unchanged by moving isolated vertices between parts or by deleting isolated vertices from the graph.

Observe Lemma 1.4.8 establishes it is enough to consider graphs without isolated vertices. For such graphs, in any optimal partition, Lemma 1.6.5 shows there is no part consisting of a single vertex and Lemma 1.6.1 shows each part must induce a connected subgraph in the original graph.

1.5 Graph properties and modularity

This section examines the behaviour of modularity with respect to the graph property of Hamiltonicity and to the graph parameter bisection width. Both these results help to give likely lower bounds for the maximum modularity of random regular graphs in Theorem 5.2.1. Other graph parameters and their influence on modularity are studied in later chapters. These parameters include treewidth in Lemma 3.2.2, distortion in Corollary 4.3.2 as well as isoperimetric graph parameters including edge expansion and Cheeger constant in Chapter 2.

1.5.1 Bisection width

In this subsection we briefly define the bisection width and give a short lemma which provides a lower bound on the modularity in terms of the bisection width.

Definition 1.5.1 (bisection width bw(G))**.** *The bisection width of a graph G, denoted* bw(G)*, is defined by*

$$\mathrm{bw}(G) = \min_{|U|=\lfloor \frac{n}{2} \rfloor} \{e(U, V \backslash U)\}.$$

Hence the bisection width gives the number of edges between parts in some partition of our vertex set into two equal or near-equal sized pieces, and thus a lower bound on modularity.

Lemma 1.5.1. *Let G be an r-regular graph G on n vertices for some positive integer r. Then*

$$q^*(G) \geq \begin{cases} \dfrac{1}{2} - 2\dfrac{\mathrm{bw}(G)}{rn} & n \text{ even} \\ \dfrac{1}{2} - 2\dfrac{\mathrm{bw}(G)}{rn} - \dfrac{1}{2n^2} & n \text{ odd.} \end{cases}$$

Proof. This is merely checking. By assumption there is a bipartition of $V(G)$ into V_1, V_2 such that $e(V_1, V_2) = \mathrm{bw}(G)$ and $|V_1| \leq |V_2| \leq |V_1| + 1$. Let $\mathcal{A} = \{V_1, V_2\}$. We can then calculate the edge contribution. Write $m = e(G)$

$$q^E_{\mathcal{A}}(G) = \frac{1}{m}(m - e(V_1, V_2)) = 1 - 2\frac{\mathrm{bw}(G)}{rn}.$$

To calculate the degree tax there are two cases depending on the parity of the number of vertices. If $n = 2h$, then $q^D_{\mathcal{A}}(G) = (\frac{h}{2h})^2 + (\frac{h}{2h})^2 = 1/2$. If $n = 2h + 1$, then $q^D_{\mathcal{A}}(G) = (\frac{h}{2h+1})^2 + (\frac{h+1}{2h+1})^2 = 1/2 + 1/(2n^2)$. This gives the required result. □

1.5.2 Hamiltonicity

The presence of a Hamilton cycle in a regular graph implies a lower bound on the maximum modularity.

Lemma 1.5.2. *Let G be a r-regular Hamiltonian graph G on n vertices for some positive integer r. Then*

$$q^*(G) \geq \frac{2}{r} + O\big(n^{-\frac{1}{2}}\big).$$

Proof. Construct a vertex partition $\mathcal{A}$, which follows the Hamilton cycle H, and breaks it into $k > 1$ parts of almost balanced sizes. Write $a = n \mod k$. Then

$$\begin{aligned} q(G) &\geq q^E_{\mathcal{A}}(G) - q^D_{\mathcal{A}}(G) \\ &\geq q^E_{\mathcal{A}}(H)\frac{e(H)}{e(G)} - q^D_{\mathcal{A}}(G) \\ &= \frac{2}{r} - \frac{k}{e(G)} - a\left(n^{-1}\lceil nk^{-1}\rceil\right)^2 - (k-a)\left(n^{-1}\lfloor nk^{-1}\rfloor\right)^2 \\ &= \frac{2}{r} - \frac{2k}{rn} - \frac{1}{k} + O\left(\frac{1}{n}\right) \end{aligned}$$

Choose $k \sim \sqrt{n}$, for example, and we have the required result. □

A result of Robinson and Wormald that almost all r-regular graphs have a Hamilton cycle for $r \geq 3$ (cubic [57] and general case [58]). This combined with our lemma above will allow us to derive some lower bounds on the modularity of random regular graphs in Theorem 5.2.1.

1.6 Further properties of the modularity function

Here we survey and develop results on the modularity function. The behaviour of the function is somewhat unintuitive at first so it can be instructive to have a collection of results on it.

We will make use of these elementary properties in later chapters as we explore the maximum modularity or likely maximum modularity for graphs with certain properties or those generated from random models.

1.6.1 Properties of optimal partitions

We are interested in the maximum modularity of graphs so it is important to establish properties of the vertex partitions which achieve this maximum modularity. This section surveys past results in [13] and adds a new definition, partial modularity, and two new observations Lemmas 1.6.2 and 1.6.5.

The following was first observed by Brandes et al. and forms Lemma 3.4 of their paper [13].

Lemma 1.6.1 (Brandes et al. [13])**.** *Let G be a graph. Then there is a vertex partition $\mathcal{A}$ of maximal modularity such that for each part $A \in \mathcal{A}$, the restriction of G to the vertices of A is a connected graph.*

To see this, let $\mathcal{A}$ be an optimal partition of G. We may move any isolated vertex into a single part of the partition as they are irrelevant (Lemma 1.4.8). If still some part induces a disconnected subgraph H then splitting this part into the vertex sets of the components of H will not change the edge contribution but will strictly decrease the degree tax.

Lemma 1.6.1 motivates us to make the following definition.

Definition 1.6.1 (partial modularity)**.** *Let G be a graph with at least s edges and $\mathcal{A}$ a vertex partition of G. Then define the partial modularity of partition $\mathcal{A}$,*

$$q_{\mathcal{A}}(G,s) = \frac{1}{s}\sum_{A\in\mathcal{A}} e(A) - \frac{1}{4s^2}\sum_{A\in\mathcal{A}} \mathrm{ds}(A)^2,$$

and the maximum partial modularity,

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

If you track the vertices of a connected component H, by the parts into which they are partitioned (in any optimal partition) each part will not contain vertices from other connected components in the graph (ignoring isolated vertices). Thus to determine how a particular connected component will be split in an optimal partition, we only need to consider the number of edges in the rest of the graph, and not the structure. Hence the following lemma.

Lemma 1.6.2. *Let G be a graph on m edges with connected components $H_0, \dots, H_l$. Then*

$$q^*(G) = \sum_{i=0}^{l} q^*(H_i, m).$$

We will use the notation of partial modularity extensively in Chapter 6 on Erdős-Rényi random graphs. The technical result, Lemma 3.2.2, tells us the partial modularity of a graph with small excess and we use this to bound the likely partial modularity of the young giant component and hence the likely maximum modularity of the random graph itself in Theorems 6.2.14 and 6.2.15.

Recall Lemma 1.4.8 stated that the placement of the isolated vertices in a partition does not affect the modularity achieved by that partition. We thus know that the placement of isolated vertices does not affect modularity. Brandes et al. also showed that, excepting these isolated vertices, every part in any optimal partition will be connected (Corollary 3.5 of [13]).

Lemma 1.6.3 (Brandes et al. [13])**.** *Suppose we have a graph G with isolated vertices $V_0 = \{v \in V(G) \ : \ deg(v) = 0\}$. Then in any optimal partition $\mathcal{A}$, $A \backslash V_0$ is connected $\forall A \in \mathcal{A}$.*

The last result of Brandes et al. which we will survey says that any node with degree 1 will not be alone in any optimal partition of our graph (Lemma 3.3 of [13]). We extend this statement to any node of non-zero degree.

Lemma 1.6.4 (Brandes et al. [13])**.** *Let G be a graph and $\mathcal{A}$ an optimal vertex partition of G. Then $A = \{u\}$ for some $A \in \mathcal{A}$ implies $deg(u) \neq 1$.*

A bit more is true. If a single vertex is a part in an optimal partition of G then it must have degree of 0.

Lemma 1.6.5. *Let G be a graph and $\mathcal{A}$ an optimal vertex partition of G. Then $A = \{u\}$ for some $A \in \mathcal{A}$ implies $deg(u) = 0$.*

Proof. Let u be a vertex with degree $d > 0$ and suppose (for a contradiction) that $\mathcal{A} = \{\{u\}, A_1, \ldots, A_k\}$ is an optimal partition of G. For each $\ell = 1, \ldots, k$ write $d_\ell = e(\{u\}, A_\ell)$ and $w_\ell = \mathrm{ds}(A_\ell)$ and define the vertex partition $\mathcal{B}_\ell = \{A_1, \ldots, A_{\ell-1}, A_\ell \cup \{u\}, \ldots, A_k\}$. We can derive a simple expression for $q_{\mathcal{B}_\ell}(G) - q_{\mathcal{A}}(G)$ as most terms cancel -

$$q_{\mathcal{B}_\ell}(G) - q_{\mathcal{A}}(G) = \frac{1}{m} e(\{u\}, A_\ell) - \frac{1}{2m^2} \deg(u)\mathrm{ds}(A_\ell) = \frac{d_\ell}{m} - \frac{dw_\ell}{2m^2}. \qquad (1.10)$$

By assumption, $\mathcal{A}$ is an optimal partition so $q_{\mathcal{B}_\ell}(G) \leq q_{\mathcal{A}}(G)$ and hence $2md_\ell \leq dw_\ell$ for each ℓ. Hence we can sum over $\ell = 1, \ldots, k$ and the inequality should hold. However $2m \sum_\ell d_\ell = 2md$ and

$$d \sum_{\ell=1}^{k} w_\ell = d \sum_{\ell=1}^{k} \mathrm{ds}(A_\ell) = d(2m - d) < 2md$$

and so we have our contradiction. □

The results of [13] together with Lemma 1.6.5 mean that the search for an optimal partition can be restricted to those in which all parts are connected subgraphs and no part consists of a single node.

1.6.2 Resolution limit of modularity

Modularity has the following peculiar property. Any connected subgraph H in a graph G, but disjoint from the rest of G, will not be split into multiple parts in any optimal partition provided that the graph G has sufficiently more edges than the subgraph H. Thus, although, H considered on its own may have a very clear community structure which begs a division into a number of pieces, it will be left undivided in any optimal partition if G has very many edges.

This lack of resolution was originally noted by Fortunato and Barthélemy [24] and identifies an important shortcoming of the modularity function. In their paper they show a canonical example of a connected graph which would usually split into two components but will remain unsplit if placed in a graph with too many edges. We state an explicit bound on how many edges are needed for general graphs to remain unsplit and also consider the option not to split versus the option to split G into *any* partition (not just bipartitions).

Example 1.6.6 (Fortunato, Barthémy [24])**.** *Suppose we have a graph G and with a connected component H which consists of the graphs K_a and K_b joined by an edge. If $e(G) \geq a^2b^2$ then in any optimal partition of G the subgraph H will remain as a connected component and not be split into K_a and K_b.*

Notice Example 1.6.6 shows the sensitivity of very large graphs to a single edge. If the complete graphs K_a and K_b were not joined by an edge then in any optimal partition they would be placed in two separate parts.

We generalise Example 1.6.6 and show that any connected component H will be classified as the same community, i.e. be included in the same part in any optimal partition, so long as the number of edges in the graph is greater than a function of the number of edges in H. Intuitively, small connected components remain unsplit.

Lemma 1.6.7. *Let G be graph with m edges, no isolated vertices and connected component H. If $e(H) < \sqrt{2m}$ then for any optimal partition $\mathcal{A}$ of G there must be some part $A \in \mathcal{A}$ such that $A = V(H)$.*

Proof. As H is disjoint from $G \backslash H$ it suffices to consider the partial modularity of H. We compare the partial modularity of taking the vertices of H to be all in the same part to the partial modularity of any partition which splits the vertices of H.

Let $\mathcal{A} = \{V(H)\}$. Write $h = e(H)$, then

$$q_{\mathcal{A}}(H, m) = \frac{h}{m} - \frac{h^2}{m^2}.$$

The best possible split into $k \geq 2$ pieces we could hope for would have $k - 1$ edges between parts and each part would have the same degree sum. Let $\mathcal{B}_k$ be any partition of $V(H)$ with k (non-empty) parts. Then for $k \geq 2$,

$$q_{\mathcal{B}_k}(H, m) \leq \frac{h - k + 1}{m} - \frac{h^2}{km^2}.$$

Hence it is strictly better not to split into $k \geq 2$ pieces if $h < \sqrt{2m}$ and we are done. □

Call the vertex partition which takes its parts to be the vertex sets of the connected components of the graph the connected components partition. In Erdős-Rényi random graphs we investigte for which edge probability p the connected components partition achieves maximum modularity. We will use Lemma 1.6.7 to prove a range of p for which it is optimal in Theorem 6.1.5.

1.6.3 Bounds on the degree tax

This section is devoted to presenting two bounds on the degree tax i.e. the bit that is subtracted away in the expression for modularity. By definition, see p14, a graph has high modularity, regarded as indicating a highly clustered graph, if it has a partition with large edge contribution and small degree tax. We recall that for a graph G with $m \geq 1$ edges and vertex partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ the degree tax is

$$q^D_{\mathcal{A}}(G) = \frac{1}{4m^2} \sum_{i=1}^{k} \mathrm{ds}(A_i)^2,$$

where $\mathrm{ds}(A_i)$ denotes the sum of the degrees of the vertices in A_i, i.e. twice the number of internal edges in A_i plus the number of edges with one endpoint in A_i.

For a graph G with with vertex partition $\mathcal{A}$ we prove an upper bound in terms of the maximal degree sum of any part in $\mathcal{A}$ (Lemma 1.6.8) and repeat a result of Brandes et al. [13] which gives a lower bound in terms of the number of parts in $\mathcal{A}$ (Lemma 1.6.10). Lemma 1.6.8 is used heavilty in Chapter 6 which is on Erdős-Rényi random graphs.

Lemma 1.6.8. *Let G be a graph with m edges and vertex partition $\mathcal{A}$. If $\max_{A \in \mathcal{A}} \mathrm{ds}(A) \leq t$ then $q^D_{\mathcal{A}}(G) \leq t/2m$.*

The proof of Lemma 1.6.8 follows by Karamata's inequality. To state this inequality we need the notion of majorisation.

Definition 1.6.2 (Majorisation)**.** *For two k-tuples of non-negative reals, we say $(y_1, \ldots, y_k)$* majorises *$(x_1, \ldots, x_k)$ if $\sum_{i=1}^k y_i = \sum_{i=1}^k x_i$ and after relabelling both tuples in descending order the inequality $\sum_{i=1}^j y_i \geq \sum_{i=1}^j x_i$ holds for each $j = 1, \ldots, k-1$.*

We can now state Karamata's inequality. This inequality, also referred to as the majorisation inequality, holds more generally for any convex function but we will only need the special case of squares, as below. Karamata's original paper [34] is in French, but the result can also be found, for instance, on p89 of Hardy, Littlewood and Pólya's paper on inequalities [28].

Lemma 1.6.9 (Karamata's inequality [34])**.** *If $x_1, \ldots, x_k, y_1, \ldots, y_k$ are non-negative reals such that $(y_1, \ldots, y_k)$ majorises $(x_1, \ldots, x_k)$ then*

$$\sum_{i=1}^{k} y_i^2 \geq \sum_{i=1}^{k} x_i^2.$$

Proof. (of Lemma 1.6.8) Denote the degree sums of the parts in $\mathcal{A}$, by $x_i = \mathrm{ds}(A_i)$. It is sufficient to prove that $0 \leq x_i \leq t$ and $\sum_i x_i \leq 2m$ together imply that $\frac{1}{4m^2}\sum_i x_i^2 \leq t/2m$. Note $\sum_i x_i = 2m$. Let r be the remainder when dividing $2m$ by t. Then construct the k-tuple $(t, \dots, t, r, 0, \dots, 0)$ which has $\lfloor \frac{2m}{t} \rfloor$ instances of t, one instance of r and enough zeroes to form a k-tuple. This tuple majorises $(x_1, \dots, x_k)$. Hence by Karamata's inequality

$$\sum_{i=1}^{k} x_i \leq \lfloor \frac{2m}{t} \rfloor t^2 + r^2 \leq 2mt,$$

and thus $\frac{1}{4m^2}\sum_{i=1}^{k} x_i^2 \leq t/2m$, as required. □

We have now proved our upper bound on the degree tax and finish this section by presenting the lower bound on the degree tax proved by Brandes et al. which appears as Corollary 6.4 in [13].

Lemma 1.6.10 (Brandes et al. [13])**.** *For any graph G with $m \geq 1$ edges and any vertex partition $\mathcal{A} = \{A_1, \dots, A_k\}$,*

$$q^D_{\mathcal{A}}(G) \geq \frac{1}{k}.$$

Observe Lemma 1.6.10 can also be proved by Karamata's inequality. Let a be the arithmetic mean of the degree sums of $\mathcal{A}$. Then $(\mathrm{ds}(A_1), \dots, \mathrm{ds}(A_k))$ majorises $(a, \dots, a)$ and $\sum_i \mathrm{ds}(A_i)^2 \geq ka^2 = (2m)^2/k$ as required.

1.6.4 Approximating maximum modularity

In this section we show that the maximum modularity can be approximated by a vertex partition with few parts. We prove that there is a partition $\mathcal{A}$ which is within $2/k$ of the optimal modularity and has only k parts.

Lemma 1.6.11. *Let G be a graph with at least one edge and let k be a positive integer. Then*

$$|q^*(G) - \max_{|\mathcal{A}| \leq k} q_{\mathcal{A}}(G)| < 2/k.$$

Proof. Suppose $\mathcal{A} = \{A_1, \ldots, A_j\}$ is an optimal vertex partition which is labeled in order of decreasing degree sum. If $\text{ds}(A) \geq 2m/k$ for each $A \in \mathcal{A}$ then $|\mathcal{A}| \leq k$ and we are done, so we suppose not. Let ℓ the largest index such that $\text{ds}(A_\ell) \geq 2m/k$. Let $\mathcal{B} = \{B_1, \ldots B_h, R\}$ be a vertex partition such that $B_i = A_i$ for $i \leq \ell$, $2m/k \leq \text{ds}(B_i) < 4m/k$ for $\ell < i \leq h$, $\text{ds}(R) < 4m/k$ and $\mathcal{A}$ refines $\mathcal{B}$. Observe that by construction $|\mathcal{B}| \leq k$ and so it is sufficient to show $q_{\mathcal{A}}(G) - q_{\mathcal{B}}(G) \leq 2/k$.

As $\mathcal{A}$ refines $\mathcal{B}$ the edge contribution of $\mathcal{B}$ will be at least that of $\mathcal{A}$ so we can bound the decrease in modularity in terms of the increase in the degree tax, i.e. $q_{\mathcal{A}}(G) - q_{\mathcal{B}}(G) \leq q^D_{\mathcal{B}}(G) - q^D_{\mathcal{A}}(G)$ which in turn simplifies further.

$$\begin{aligned} q^D_{\mathcal{B}}(G) - q^D_{\mathcal{A}}(G) &= \frac{1}{4m^2}\left(\sum_{i>j} \text{ds}(B_j)^2 + \text{ds}(R)^2 - \sum_{i>j} \text{ds}(A_j)^2\right) \\ &\leq \frac{1}{4m^2}\left(\sum_{i>j} \text{ds}(B_j)^2 + \text{ds}(R)^2\right). \qquad (1.11) \end{aligned}$$

By Karamata's inequality, Lemma 1.6.9, the sum of squares in (1.11) is maximised if there are $k/2$ parts each with degree sum $4m/k$ and thus (1.11) $\leq k/2$. This completes the proof. $\square$

Chapter 2

Isoperimetric inequalities and modularity

This chapter develops upper bounds on the maximum modularity of a graph G in terms of the edge expansion and other isoperimetric properties of G.

We prove three such upper bounds. The first of these, Theorem 2.1.1, bounds the modularity of a graph in terms of an isoperimetric parameter of the graph, the Cheeger constant. The theorem is proved by an application of the probabilistic method and a 'balancing result', Lemma 2.1.3.

The second result is Theorem 2.2.1 which gives an upper bound in terms of the Cheeger constant of small vertex subsets in the graph. This will enable us to prove likely upper bounds on the modularity of random regular graphs in Theorem 5.2.1.

Lastly, Lemma 2.3.1 provides an upper bound in terms of a maximisation problem over vertex sets in the graph. This lemma is extended in Chapter 4 and used to establish the maximum modularity of an integer lattice in Theorem 4.4.1.

Some results in Section 2.1 have been published in [47]. This paper conatined Corollary 2.1.2 and Lemma 2.1.3. Also, the proof of Corollary 2.1.2 proceeded in a similar way to the proof of the more general result Theorem 2.1.1 in this thesis.

2.1 Edge expansion and modularity

The main result of this section is Theorem 2.1.1 which gives bounds on the maximum modularity of a graph in terms of an isoperimetric paramter of the graph, the Cheeger constant. We also give a corollary for regular graphs which bounds a graphs modularity in terms of its edge expansion, also known as isoperimetric number. We define these below, following the notation of [14] and [15].

Definition 2.1.1. *For a graph G with m edges define its* Cheeger constant*, $h(G)$ to be*

$$h(G) = \min_{\mathrm{ds}(U) \leq m} \frac{1}{\mathrm{ds}(U)} e(U, V \backslash U),$$

and for a graph G with n vertices define its edge expansion*, $i(G)$, to be*

$$i(G) = \min_{|U| \leq n/2} \frac{1}{|U|} e(U, V \backslash U).$$

There is an easy argument which gives a weaker version of the bound in Theorem 2.1.1. Let G be a graph with m vertices, Cheeger constant $h(G)$ and vertex partition $\mathcal{A} = (A_1, \ldots, A_k)$. Then the following upper bound on the modularity is almost immediate.

$$q_{\mathcal{A}}(G) < \max\{1 - h(G), 3/4\}. \tag{2.1}$$

There are two cases to check. (a) Suppose that each $\mathrm{ds}(A_i) \leq m$. Then the number of edges between parts in $\mathcal{A}$ is $\frac{1}{2}\sum_i e(A_i, V \backslash A_i) \geq \frac{1}{2}\sum_i \mathrm{ds}(A_i) h(G) = mh(G)$. Hence the edge contribution is at most $1 - h(G)$ and the degree tax is strictly positive so $q_{\mathcal{A}}(G) < 1 - h(G)$. (b) If say $\mathrm{ds}(A_1) > m$ then the degree tax is at least $\mathrm{ds}(A_1)^2/(4m^2) > 1/4$ and so $q_{\mathcal{A}}(G) < 3/4$.

In Theorem 2.1.1 we improve the upper bound in (2.1) to approximately $1 - 2h(G)$, when the maximum size of parts in our partition is restricted. We need new notation.

Definition 2.1.2 (restricted modularity)**.** *Define $q^*_\delta(G)$ to be the maximum modularity of $q_{\mathcal{A}}(G)$ over all partitions $\mathcal{A}$ in which each part has* $\mathrm{ds}(A) \leq 2\delta m$.

Observe that for G a regular graph, $q^*_\delta(G)$ is the maximum modularity of $q_{\mathcal{A}}(G)$ over all partitions $\mathcal{A}$ in which each part has size $|A| \leq \delta n$.

Theorem 2.1.1. *Let G be a graph with at least $\delta^{-1}/2$ edges. Then*

$$q^*_\delta(G) < 1 - 2h(G)(1 + \sqrt{\delta} + 2\delta) + \sqrt{\delta}.$$

Consider the important special case of a regular graph. If G is regular then the condition $\mathrm{ds}(U) \le m$ is equivalent to $|U| \le n/2$. Hence, observing $\mathrm{ds}(U) = r|U|$, for an r-regular graph G, $h(G) = i(G)/r$. Hence the following is a corollary of Theorem 2.1.1.

Corollary 2.1.2. *Let G be an r-regular graph with at least δ^{-1} vertices. Then*

$$q^*_\delta(G) < 1 - \frac{2i(G)}{r}(1 + \sqrt{\delta} + 2\delta) + \sqrt{\delta}.$$

The proof of Theorem 2.1.1 hinges on the following lemma, which we will state and prove before returning to the proof of our theorem.

Lemma 2.1.3. *Fix positive integers t and n, and consider the complete graph K_n on the vertex set $1, \ldots, n$ with non-negative vertex weights such that $w(1) \ge w(2) \ge \ldots \ge w(n)$. Let $\mathcal{M}$ be a perfect matching on K_n such that $|a - b| \le t$ for each edge $ab \in \mathcal{M}$. Construct a red-blue (improper) vertex-colouring c of K_n by colouring one end of each edge in $\mathcal{M}$ red and the other end blue. Then*

$$\Big| \sum_{v\colon c(v) \text{ red}} w(v) - \sum_{u\colon c(u) \text{ blue}} w(u) \Big| \le t\,(w(1) - w(n)). \tag{2.2}$$

Proof. Observe that the left side of (2.2) is at most

$$\sum_{ab\in\mathcal{M},\, a<b} (w(a) - w(b)) = \sum_{j=1}^{n-1} (w(j) - w(j+1))n_j$$

where n_j is the number of distinct edges $ab \in \mathcal{M}$ with $a < b$ such that $j, j+1 \in \{a, \ldots, b\}$. Let $ab \in \mathcal{M}$ with $a < b$, and let $j \in \{a, \ldots, b\}$. Then $a \in \{j - t, \ldots, j\}$ and $b \in \{j, \ldots, j+t\}$, since otherwise either $a \le j-(t+1)$ and $b \ge j$, or $b \ge j+t+1$ and $a \le j$, and so $b-a \ge t+1$. Thus if $ab \in \mathcal{M}$ then $a, b \in \{j - t, \ldots, j + t\}$. Hence, if we had $j \in \{a, \ldots, b\}$ for at least $t + 1$ distinct edges $ab \in \mathcal{M}$ with $a < b$ then all $2t + 2$ end vertices involved would have to be in the set $\{j - t, \ldots, j + t\}$ of $2t + 1$ vertices, a contradiction. It follows that each $n_j \le t$, and so

$$\sum_{j=1}^{n-1} (w(j) - w(j+1))n_j \le t \cdot \sum_{j=1}^{n-1} (w(j) - w(j+1)) = t\,(w(1) - w(n)).$$

which completes the proof. □

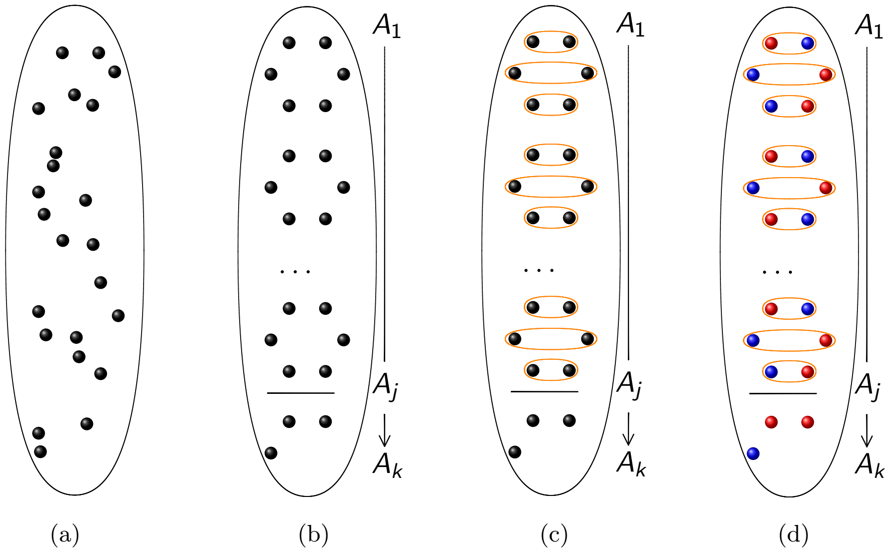


Figure 2.1: An illustration of the steps in the proof of Theorem 2.1.1.
(a). Depicts the vertex partition $\mathcal{A}$. The parts $A_1, \ldots, A_k$ are shown as black dots.
(b). We rearrange the parts into groups of size $t + 1 = 6$ in order of decreasing degree sums $\text{ds}(A_1) \geq \ldots \geq \text{ds}(A_k)$. As the number of parts is not a multiple of six, we have some remnants.
(c). The complete graph K_6 decomposes into edge disjoint perfect matchings as in Figure 2.2. Each perfect matching in K_6 induces a matching on the parts of $\mathcal{A}$ such that each part is paired to another part within the same group of six i.e. of similar degree sum. We choose the perfect matching of K_6, say orange, which induces the least number of edges between paired parts.
(d). Independently for each pair of parts, we uniformly choose one to be blue and one red. Unpaired parts are coloured red or blue with probability one half.

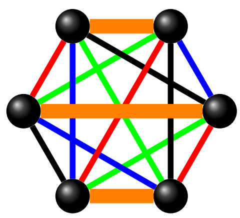


Figure 2.2: The complete graph on six vertices, K_6, decomposed into perfect matchings.

Proof. (of Theorem 2.1.1). Proof outline. Given a partition $\mathcal{A}$, we pair up the parts, and then (randomly) divide the parts into two groups by placing one part from each pair in each group. Let U be the vertices in the parts of the first group and V the rest. We use Lemma 2.1.3 to ensure that U and V have approximately equal degree sums. There are sufficiently many pairings available that we can ensure that there are not many edges between each pair of parts. The Cheeger constant of our graph then gives us a lower bound on the expected number of edges between U and V, and hence an upper bound for the modularity. See Figure 2.1 on p54 for an illustration.

Let $t = t(\delta)$ be an odd integer whose value we will set later. Let $\mathcal{A} = \{A_1, \ldots, A_k\}$ be any partition of G such that $2\delta m \geq \mathrm{ds}(A_1) \geq \cdots \geq \mathrm{ds}(A_k)$.

Recall that the edge set of a complete graph on an even number of vertices has a decomposition into perfect matchings (see Figure 2.2 for an example). Let $\{\mathcal{M}_\alpha\}_{\alpha=1}^{t}$ be a set of edge disjoint perfect matchings in K_{t+1}. To avoid parity problems when $t+1 \not| k$, set $k' = k'(n) = \lfloor k/(t+1) \rfloor (t+1)$ and let $Q = \{k'+1, \ldots, k\}$. For each matching $\mathcal{M}_\alpha$ we define a pairing $\mathcal{P}_\alpha$ on the parts $A_1, \ldots, A_{k'}$ in our partition $\mathcal{A}$. For $1 \leq i \neq j \leq k'$,

$$\{i,j\} \in \mathcal{P}_\alpha \;\Leftrightarrow\; uv \in E(\mathcal{M}_\alpha),\; \left\lfloor \tfrac{i}{t+1} \right\rfloor = \left\lfloor \tfrac{j}{t+1} \right\rfloor,\; \begin{array}{c} i = u \pmod{t+1} \\ j = v \pmod{t+1} \end{array}. \tag{2.3}$$

We choose a perfect matching $\mathcal{M}_\alpha$ that minimises the total number of edges between A_i and A_j for the pairs $\{i,j\} \in \mathcal{P}_\alpha$. Let $E_\alpha = \cup_{\{i,j\}\in\mathcal{P}_\alpha} E(A_i, A_j)$ and set $\alpha' = \arg\min |E_\alpha|$. Then $|E_{\alpha'}| \leq m/t$.

Now construct a random bipartition of the parts of $\mathcal{A}$: $\forall\ \{i,j\} \in \mathcal{P}_{\alpha'}$ add A_i to U and A_j to V with probability $\frac{1}{2}$ and add A_i to V and A_j to U otherwise, and $\forall h \in Q$, add A_h to U with probability $\frac{1}{2}$ and to V otherwise. Now, because $|i-j| \leq t$, $\forall \{i,j\} \in \mathcal{P}_{\alpha'}$ (which means Lemma 2.1.3 applies with $w(i) = \mathrm{ds}(A_i)$) and $|Q| \leq t$,

$$|\mathrm{ds}(U) - \mathrm{ds}(V)| \leq t(\mathrm{ds}(A_1) - \mathrm{ds}(A_{k'})) + t\mathrm{ds}(A_{k'+1}) \leq t\mathrm{ds}(A_1).$$

Thus $\mathrm{ds}(U), \mathrm{ds}(V) \geq m - \frac{t}{2}\mathrm{ds}(A_1)$. Hence by the definition of the Cheeger constant, for any bipartition $e(U,V) \geq h(G)(m - t\mathrm{ds}(A_1)/2)$ and so

$$\mathbb{E}(e(U,V)) \geq h(G)(m - t\mathrm{ds}(A_1)/2). \tag{2.4}$$

By construction of our random bipartition, any edge between non-paired parts has probability one half to be between the random sets U and V. We denote this set of edges by

$E_\beta = \big(\cup_{i \neq j} E(A_i, A_j)\big) \backslash E_{\alpha'}$, so if $e \in E_\beta$, then $\mathbb{P}(e \in E(U,V)) = 1/2$. Note also that for $e \in E_{\alpha'}$, $\mathbb{P}(e \in E(U,V)) = 1$. Thus

$$\mathbb{E}(e(U,V)) = \frac{1}{2}|E_\beta| + |E_{\alpha'}|. \tag{2.5}$$

Recall the definition of modularity implies,

$$q_{\mathcal{A}}(G) \leq q^E_{\mathcal{A}}(G) = \tfrac{1}{m} \textstyle\sum_{A \in \mathcal{A}} E(A) = 1 - \tfrac{1}{m}\big(|E_{\alpha'}| + |E_\beta|\big). \tag{2.6}$$

We rearrange (2.5) and then apply our inequality (2.4),

$$|E_\beta| + |E_{\alpha'}| = 2\mathbb{E}(e(U,V)) - |E_{\alpha'}| \geq h(G)(2m - t\mathrm{ds}(A_1)) - \tfrac{m}{t}. \tag{2.7}$$

Recall $\mathrm{ds}(A_1) \leq 2\delta m$ hence by (2.6) and (2.7),

$$q_{\mathcal{A}}(G) \leq 1 - 2h(G)(1 + \delta t) + \frac{1}{t}. \tag{2.8}$$

Finally observe that we can set t to be the outcome of rounding $\sqrt{\delta^{-1}}$ up to the nearest odd integer to complete the proof. $\square$

2.2 Edge expansion of small sets

For this section we define the u-Cheeger constant of a graph, as a minimum over the same expression as for the Cheeger constant but restricting to bipartitions in which the degree sum of one of the parts is at most $2um$. Likewise the u-edge expansion restricts to bipartitions where the smaller part has no more than un vertices. For edge expansion this follows the notation of [35]. Notice that for $u = 1/2$ these reduce to the constants defined in the last section, i.e. $h_{1/2}(G) = h(G)$ and $i_{1/2}(G) = i(G)$.

Definition 2.2.1. *For a graph G with m edges define its u-*Cheeger constant*, $h_u(G)$ to be*

$$h_u(G) = \min_{\mathrm{ds}(U) \leq 2um} \frac{1}{\mathrm{ds}(U)} e(U, V \backslash U),$$

*and for a graph G with n vertices define its u-*edge expansion*, $i_u(G)$, to be*

$$i_u(G) = \min_{|U| \leq un} \frac{1}{|U|} e(U, V \backslash U).$$

We take the minimum over an empty set to be ∞ as we only want to consider non-empty sets of vertices U. It is now possible to state our theorem.

Theorem 2.2.1. *Let G be a graph with $m \geq 1$ edges. Let $\alpha < 1$, and suppose for all $0 < u \leq 1/2$ that $u + h_u(G) > \alpha$. Then*

$$q^*(G) < 1 - \alpha. \tag{2.9}$$

Consider again the special case of a regular graph. If G is r-regular then the condition $\mathrm{ds}(U) \leq 2um$ is equivalent to $|U| \leq un$ and $\mathrm{ds}(U) = r|U|$. Hence for an r-regular graph G, $h_u(G) = i_u(G)/r$, and we get the following corollary of Theorem 2.2.1.

Corollary 2.2.2. *Let G be an r-regular graph with $m \geq 1$ edges. Let $\alpha < 1$, and suppose for all $0 < u \leq 1/2$ that $u + i_u(G)/r > \alpha$. Then*

$$q^*(G) < 1 - \alpha. \tag{2.10}$$

This corollary together with a result of Kolesnik and Wormald [35] will enable us to prove an upper bound for the modularity of a random cubic graph. This is done in Theorem 5.2.1 on p94.

Proof. We fix a vertex partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ and show $q_{\mathcal{A}}(G)$ satisfies (2.9). Note we can calculate $1 - q^E_{\mathcal{A}}(G)$ by summing the number of edges leaving each part and dividing by two (as we double counted each of these edges). Thus, letting $u_j = \text{ds}(A_j)/2m$,

$$\begin{aligned} 1 - q_{\mathcal{A}}(G) &= 1 - q^E_{\mathcal{A}}(G) + q^D_{\mathcal{A}}(G) \\ &= \tfrac{1}{2m} \sum_j e(A_j, V \backslash A_j) + \tfrac{1}{4m^2} \sum_j \text{ds}(A_j)^2 \\ &= \sum_j u_j e(A_j, V\backslash A_j)/\text{ds}(A_j) + \sum_j u_j^2. \end{aligned} \tag{2.11}$$

We will show (2.11) is at most α. There are two cases as the proof is dependent on the degree sum of the largest part in $\mathcal{A}$. First suppose that $u_i \leq 1/2 \ \forall i$. We can now substitute $h_{u_j}(G)$ as a lower bound for $e(A_j, V\backslash A_j)/\text{ds}(A_j)$. Then

$$\begin{aligned} 1 - q_{\mathcal{A}}(G) &\geq \sum_j u_j h_{u_j}(G) + \sum_j u_j^2 \\ &= \sum_j u_j (h_{u_j}(G) + u_j) \\ &> \alpha \sum_j u_j = \alpha, \end{aligned}$$

as required. For the second case, if say $u_1 > 1/2$, we start by observing a simple rearrangement of (2.11),

$$1 - q_{\mathcal{A}}(G) = (1-u_1) e(A_1, V\backslash A_1)/\text{ds}(V\backslash A_1) + \sum_{j>1} u_j e(A_j, V\backslash A_j)/\text{ds}(A_j) + \sum_{j\geq 1} u_j^2.$$

Now because $u_1 > 1/2$, the relevant inequality bounding the number edges leaving A_1 in terms of our Cheeger constant is $e(A_1, V\backslash A_1) \geq h_{1-u_1}(G)\text{ds}(V\backslash A_1)$.

$$1 - q_{\mathcal{A}}(G) \geq (1-u_1) h_{1-u_1}(G) + u_1^2 + \sum_{j>1} u_j (h_{u_1}(G) + u_j).$$

This can be rearranged,

$$\begin{aligned} 1 - q_{\mathcal{A}}(G) &\geq (1-u_1)(h_{1-u_1}(G) + (1-u_1)) - (1-u_1)^2 + u_1^2 + \sum_{j>1} u_j (h_{u_1}(G) + u_j). \\ &= (1-u_1)(h_{1-u_1}(G) + (1-u_1)) + 2u_1 - 1 + \sum_{j>1} u_j (h_{u_1}(G) + u_j). \\ &> \alpha(1-u_1) + 2u_1 - 1 + \alpha \sum_{j>1} u_j. \\ &= \alpha + (2u_1 - 1)(1-\alpha). \\ &> \alpha \end{aligned}$$

and we are done. The last inequality holds because $2u_1 > 1$ and $\alpha < 1$. □

2.3 Modularity as a function of the best vertex set

We show that the modularity of a regular graph G, can never be better than a certain maximisation problem over vertex subsets of G. Note this expresses a bound for modularity, which is a function of vertex partitions, as a function over individual vertex subsets of G.

Lemma 2.3.1. *Let G be a graph with m edges. Then*

$$q^*(G) \leq \max_{A \subseteq V(G)} \left(\frac{2e(A)}{\mathrm{ds}(A)} - \frac{\mathrm{ds}(A)}{2m} \right),$$

and let G be a regular graph with m edges and n vertices. Then

$$q^*(G) \leq \max_{A \subseteq V(G)} \left(\frac{e(A)n}{|A|m} - \frac{|A|}{n} \right).$$

Proof. We first establish that the regular case follows from the general one. Suppose G is an r-regular graph. Then $m = rn/2$ and

$$\frac{2e(A)}{\mathrm{ds}(A)} = \frac{2e(A)}{|A|r} = \frac{e(A)n}{|A|m}.$$

Likewise

$$\frac{\mathrm{ds}(A)}{2m} = \frac{|A|r}{rn} = \frac{|A|}{n}.$$

Hence it suffices to prove the general case. Fix an optimal vertex partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ and write $a_i = \mathrm{ds}(A_i)/(2m)$. Then rearrange the expression for modularity:

$$q^*(G) = q_{\mathcal{A}}(G) = \sum_i \left(\frac{e(A_i)}{m} - \left(\frac{\mathrm{ds}(A_i)}{2m} \right)^2 \right) = \sum_i a_i \left(\frac{e(A_i)}{a_i m} - a_i \right). \tag{2.12}$$

As $\sum_i a_i = 1$, line (2.12) allows us to write an upperbound in terms of a single vertex part in $\mathcal{A}$

$$q_{\mathcal{A}}(G) \leq \max_i \left(\frac{e(A_i)}{a_i m} - a_i \right) \leq \max_{A \subseteq V(G)} \left(\frac{2e(A)}{\mathrm{ds}(A)} - \frac{\mathrm{ds}(A)}{2m} \right).$$

□

We use an extension of Lemma 2.3.1, namely Lemma 4.4.4, to prove upper bounds for the modularity of a 'near'-regular graph in Theorem 4.4.1.

Chapter 3

Trees and tree-like graphs

This chapter proves lower bounds on the maximum modularity of trees and tree-like graphs with low degree. We briefly review previous results, see p23 for further details. Bagrow makes a study of the modularity of some trees and tree-like graphs in [2]. He shows Galton-Watson trees and k-ary trees have modularity tending to one. In [16] 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 tree width. This forms Theorem 3.1.1. We develop a technical result, Lemma 3.2.2, which will later help us partition the giant component in Erdős-Rényi random graphs in Section 6.2.3, p119.

3.1 Trees and graphs with low tree width

Let us recall the definition of treewidth: see [5] for a survey.

Definition 3.1.1 (treewidth, tw)**.** *A* tree-decomposition *of a graph $G = (V, E)$ is a pair $(\{X_i|i \in I\}, T = (I, F))$ with $\{X_i|i \in I\}$ a family of subsets of V, one for each node of T, and T a tree, such that*

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

2. $\forall vw \in E$, $\exists i \in I$ *such that* $v, w \in X_i$*.*

3. $\forall i, j, k \in I$*: if j is on the path from i to k in T, then* $X_i \cap X_k \subseteq X_j$*.*

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

It is now possible to state our results. The proof of Theorem 3.1.1 is deferred until p66.

Theorem 3.1.1. *Let G be a graph with $m \geq 1$ edges, treewidth $\mathrm{tw}(G) = t$ and maximum degree $\Delta = \Delta(G)$. Then the modularity $q^*(G)$ satisfies*

$$q^*(G) \geq 1 - 2((t+1)\Delta/m)^{1/2}.$$

Remark. Let C_m be the cycle with m edges. The modularity is $q^*(C_m) = 1 - \Theta(1/\sqrt{m})$ by Theorem 6.7 [13]. Observe cycles have both treewidth and maximum degree two and thus Theorem 3.1.1 gives the correct order of magnitude for the rate of convergence of cycles.

Corollary 3.1.2. *For $m = 1, 2, \ldots$ let G_m be a graph with m edges. If $\mathrm{tw}(G_m) \cdot \Delta(G_m) = o(m)$ then $q^*(G_m) \to 1$ as $m \to \infty$.*

The Corollary 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 $\mathrm{tw}(G) \cdot \Delta(G) = 1 \cdot m = m$ and $q^*(G) = 0$ by Theorem 1.3.5.
(b) If G is the random cubic graph $G_{n,3}$ (so $m = 3n/2$) then $\mathrm{tw}(G) \cdot \Delta(G) = 3\,\mathrm{tw}(G) = O(m)$ and $q^*(G) \leq 0.8$ whp. The upper bound on $q^*(G)$ is proved in Theorem 5.2.1, and is an improvement on the bound in [47].

The lower bound in terms of treewidth and maximum degree in Corollary 3.1.2 implies random graphs on surfaces, including random planar graphs, have asymptotically maximal modularity whp. For a surface S let $G_S(n)$ be chosen uniformly from all labelled n vertex graphs which embed into S without crossing edges. For S of bounded genus the graph G_S has $\mathrm{tw}(G_S) = O(\sqrt{n})$ by [20], [26] and whp maximum degree $\Delta(G_S) = O(\log n)$ [46] which implies the result.

Corollary 3.1.3. *Let S be a surface of bounded genus. Then whp*

$$q^*(G_S(n)) \geq 1 - O(\log n/\sqrt{n}).$$

Our theorem also provides a lower bound on the modularity of G in terms of the *separation number* of G which we denote $\mathrm{sn}(G)$. Intuitively the separation number is the smallest number of vertices one can remove from G so that the remainder of the vertices can be split into two sets of roughly equal size with no edges going from one set to the other.

Formally, let (A, B) be a *separation* of G if $A, B \subset V(G)$ and $E(A \backslash B, B \backslash A) = \varnothing$. The sets A and B can overlap and we call $|A \cap B|$ the *order* of the separation. Then $\mathrm{sn}(G)$ is the smallest s such that every subgraph of $H \subset G$ has a separation (A, B) of order at most s such that $|A \backslash B|, |B \backslash A| \leq 2|H|/3$.

Recently Dvorak and Norin proved that for all graphs G, $\mathrm{tw}(G) \leq 105\mathrm{sn}(G)$ [20]. Thus, by Theorem 3.1.1, $q(G) \geq 1 - 22(sn(G)\Delta/m)^{1/2}$.

3.2 Nearly low tree-width – a technical lemma

The motivation for our technical result, Lemma 3.2.2 is twofold. Firstly it will help in the proof of Theorem 3.1.1. However the lemma is proven in greater generality than needed for Theorem 3.1.1. The reason for including an optional set E' in the statement of the lemma is the following. For Erdős-Rényi random graphs where $p = c/n$ for constant $c > 1$ whp we have a giant component which is 'close' to a tree. This time, by close to a tree, we mean that there is a 'small' number of edges that can be deleted to leave it a tree. We can take advantage of this to find a partition of the giant component which has high partial modularity and so will extend to a high modularity partition of our random graph. This result is Lemma 3.2.2 which defines the 'prune-to-forest' construction used in Theorems 6.2.14 and 6.2.15.

The outline of this section is that we first prove Lemma 3.2.1 which lets us split a graph H into parts with certain degree sums. Using this lemma we prove our technical result, Lemma 3.2.2, and then the proof of Theorem 3.1.1 follows easily.

Lemma 3.2.1. *Let the graph H have h edges, maximum degree d and edge set $E' \in E(H)$ of size ℓ such that $H \backslash E'$ has treewidth t. Let s be an integer such that $d < s \leq 2h - d$. By deleting the edges incident with at most $t + 1$ vertices, we can find a partition $V(H) = V_0 \cup \cdots \cup V_{k-1}$ into $k \geq 3$ parts with no cross-edges in E', such that $\mathrm{ds}_H(V_0) \leq 2h - s$ and $\mathrm{ds}_H(V_i) < s$ for each $i = 1, \ldots, k-1$.*

Figure 3.1 provides an illustrated example to accompany the proof, see p67.

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

The proof will take a tree-decomposition of G, choose one bag X_i, and delete all edges of G incident to the vertices in X_i. Observe we can guarantee a tree decomposition T of G with 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 node.

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 $T \backslash e$, let V_e be the set of vertices contained in the bags of T_e, and let $d_e = w(V_e)$, the sum of the degrees in H of these vertices.

If $d_e < s$, then orient e toward the root node, otherwise, orient e away from the root node.

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

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 $k \geq 1$. If there is one such neighbour, let $V_1 = V_{ij_1}$ and $V_2 = X_i \setminus V_1$, so $w(V_1) < s$ (since the edge $j_1 i$ is oriented towards i) and $w(V_2) \leq d < s$ (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 $w(V_i) < s$ for each i. □

Repeated applications of Lemma 3.2.1 are used in the proof of our technical lemma, Lemma 3.2.2. Lemma 3.2.1 allows us construct a vertex partition of H based on the tree-decomposition of $H \backslash E'$. The construction defined in the proof of Lemma 3.2.2, $\mathcal{PF}$, we call the prune-to-forest partition and use it to prove results for random graphs in Section 6.2.3.

Lemma 3.2.2. *Let the graph H have h edges, maximum degree d and edge set $E' \in E(H)$ such that $H \backslash E'$ has treewidth t. Let $s > 2d$. Then for $r \geq h$,*

$$q_{\mathcal{PF}}(H, r) \geq \frac{h}{r} - \frac{|E'|}{r} - \frac{2h(t+1)d}{sr} - \frac{h(s-1)}{2r^2},$$

and if $d < r(t+1)$ then,

$$q_{\mathcal{PF}}(H, r) \geq \frac{h}{r} - \frac{|E'|}{r} - \frac{2h\sqrt{(t+1)d}}{r^{3/2}}.$$

Proof. Set $\tilde{H} = H$ and $\tilde{h} = e(\tilde{H})$. As long as $2\tilde{h} \geq s + d$ we use Lemma 3.2.1 repeatedly to 'break off parts' $V_1, V_2, \ldots$ and replace $\tilde{H}$ by its induced subgraph on V_0, where $w(V_0) \leq 2\tilde{h} - s$. After $j \leq 2h/s - 1$ steps we have $2\tilde{h} < s + d$. At this stage we have lost at most $j(t+1)d$ edges (not in E'), and each of the parts 'broken off' from H has weight sum $\leq s - 1$.

We **claim** we can complete this to a vertex partition, call it $\mathcal{PF}$, such that each part has weight sum at most $s - 1$ and the number of cross-edges (not in E') is at most $\frac{2h}{s}(t+1)d$.

If $2\tilde{h} \leq s-1$ we are already done, so consider the other case, when $s \leq 2\tilde{h} < s+d$. Now let $s' = s-d$, and note that $d < s' < 2\tilde{h} - d$. We can apply the lemma with s' to complete the proof of the claim, since

$$2\tilde{h} - s' < s + d - (s-d) = 2d \leq s.$$

To bound the degree tax note that $0 \leq x_i \leq s-1$ and $\sum_i x_i \leq 2h$ together imply that $\sum_i x_i^2 \leq 2h(s-1)$, and so finally, by this and the claim,

$$q_{\mathcal{PF}}(H,r) \quad \geq \quad \frac{h}{r} - \frac{|E'|}{r} - \frac{2h(t+1)d}{sr} - \frac{h(s-1)}{2r^2} \tag{3.1}$$

and this completes the first part of the proof. The second part is an application of the first. If $d < (t+1)r$ we can set $s = 2((t+1)dm)^{1/2}$ (and it satisfies $s > 2d$) then substitute this value of s into (3.1). $\square$

Having established our technical lemma the proof of the main theorem of this chapter is now straightforward.

Proof. (of Theorem 3.1.1) Write d for Δ and $m = e(G)$. Since $q^*(G) \geq 0$ for any graph G we need only prove the case where $m > 4(t+1)d$. Let $s = \lceil 2((t+1)dm)^{\frac{1}{2}} \rceil$ and note $s > 4(t+1)d$.

As $s > 2d$, we can apply Lemma 3.2.2 with $H = G$, $E' = \varnothing$ and $r = m$, then

$$q_{\mathcal{PF}}(G) \geq 1 - \frac{2(t+1)d}{s} - \frac{s-1}{2m}.$$

Hence by our choice of s, we get $q^*(G) \geq q_{\mathcal{PF}}(G) \geq 1 - 2\left((t+1)d/m\right)^{1/2}$ as required. $\square$

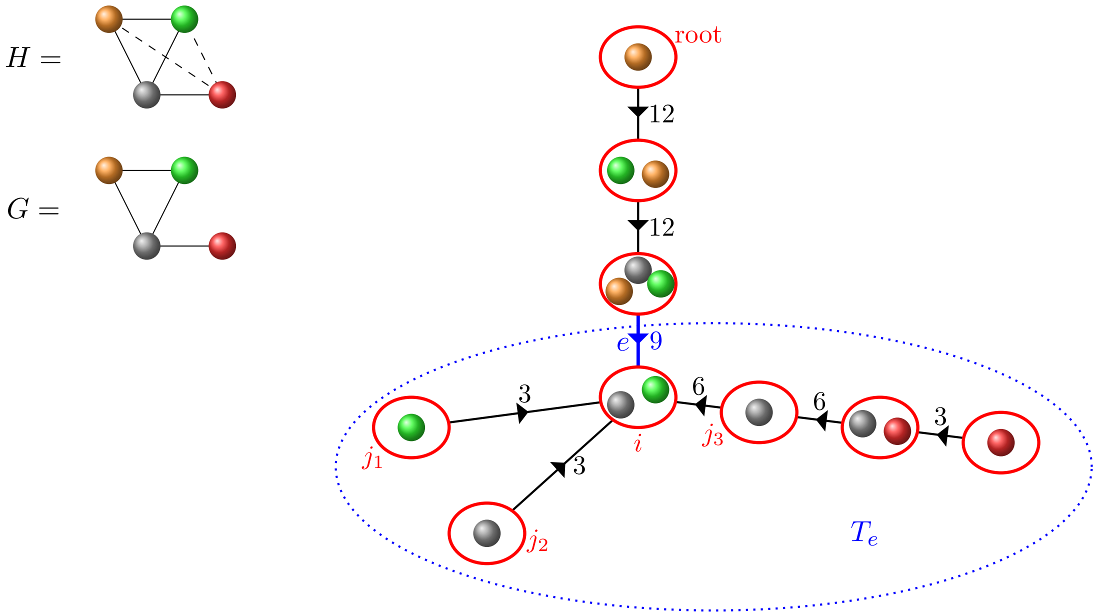


Figure 3.1: An illustration of the construction in the proof of Lemma 3.2.1 applied to a toy graph H with edge set E' (dashed) and $s = 8$. Graph H has treewidth 3 but after removing the dashed edges graph G has treewidth 2. A tree-decomposition for G is shown and the leaf node at the top chosen to be the root. For each edge h in the tree-decomposition the parameter d_h is depicted and the edge oriented toward the node if $d_h < 8$. Note this defines node i, edge e and component T_e as shown.

3.3 Optimal partitions of tree-like connected components

The structure of an optimal partition of a graph is of interest. We shall see in this section that Lemma 3.2.2 can be applied to study optimal partitions.

Recall Example 1.6.6 from earlier in the thesis. If a connected component in the graph consists of two complete graphs joined by an edge then counterintuitively they will be classified as one community instead of split in two if the number of edges in the rest of the graph is large enough. More generally, Lemma 1.6.7 showed a threshold whereby a general connected component will be classified as one community in any optimal partition if the edge count in the entire graph exceeds a certain function. For a graph G with no isolated vertices and H a connected component of G, if $e(H) < \sqrt{2e(G)}$, then in any opitimal partition $\mathcal{A}$, the vertices of H will be unsplit i.e. $V(H) = A$ for some part $A \in \mathcal{A}$.

In the next lemma we give the complementary result. We want to show a threshold so that if the number of edges in a connected component H is above this then it will be split in any optimal partition. However, we need conditions on the structure of H, for example if H is a star it will never be better to split it. Lemma 3.3.1 shows such a threshold does indeed exist if H is a 'close' to tree and has small maximum degree.

Lemma 3.3.1. *Let G be graph with m edges and a connected component H which has maximal degree $\Delta = \Delta(H)$. If H is a tree then an optimal partition will split H if $e(H) > 2\sqrt{2\Delta m}$.*

If there is a set $E' \subset E(H)$ such that $H \backslash E'$ has treewidth t then an optimal partition will split H if

$$e(H)^2 > |E'|m + 2e(H)\sqrt{(t+1)\Delta m}.$$

Proof. Write $h = e(H)$ and $\Delta = \Delta(H)$. It is enough to consider the partial modularity of H when split via the prune-to-forest construction as in Lemma 3.2.2. By that lemma,

$$q_{\mathcal{PF}}(H,m) \geq \frac{h}{m} - \frac{|E'|}{m} - \frac{2h\sqrt{2\Delta}}{m^{3/2}},$$

which compares to the partial modularity of not splitting, i.e. $\mathcal{A} = \{V(H)\}$,

$$q_{\mathcal{A}}(H,m) = \frac{h}{m} - \frac{h^2}{m^2}.$$

Thus $\mathcal{PF}$ is better than not splitting H if $\frac{|E'|}{m} + \frac{2h\sqrt{(t+1)\Delta}}{m^{3/2}} < \frac{h^2}{m^2}$. This proves the second part of the lemma. In the first part we assume H is a tree, so $E' = \varnothing$ and $t = 1$ so $\mathcal{PF}$ is strictly better if $\frac{2h\sqrt{2\Delta}}{m^{3/2}} < \frac{h^2}{m^2}$, i.e. for $h > 2\sqrt{2\Delta m}$ as claimed. □

In particular notice that one can remove a set of edges E' from H so that $H \backslash E'$ is a tree (of treewidth 1) and $|E'|$ is the excess of component H. Lemma 3.3.1 will be used in the proof of Theorem 6.1.5 which gives information on the likely structure of the optimal partitions of Erdős-Rényi graphs.

Chapter 4

Lattices and lattice-like graphs

In this chapter we show that any subgraph of the square lattice with many edges has high modularity and similarly for an integer lattice in $\mathbb{R}^d$, even with certain additional edges which might seem likely to keep the modularity low. Further we show that any graphs which can embed 'nicely' in $\mathbb{R}^d$ i.e. with a small ratio between maximum edge length and minimum vertex separation, also have high modularity. These two results form Theorem 4.2.1 and 4.3.1 respectively. Lastly we use isoperimetric results to show in Theorem 4.4.1 our upper and lower bounds for the maximum modularity of the complete integer lattice match and give an asymptotic expression for the maximum modularity.

4.1 Previous work on complete sections of lattice

The connection between the Potts model and modularity, described on p16, makes lattices a natural object to study. Our contribution builds on previous work in Statistical Physics. The modularity of particular regular lattices was investigated by Guimerà et al. [27] and by Massen and Doye [44]. We discuss these two papers.

The main thrust of [44] was to compare the performance of different algorithms on estimating modularity on example networks derived from clusters of atoms. The second part of [44] numerically investigates the value of modularity for large complete sections of the hexagonal lattices in $\mathbb{R}^2$ which they calculate to be very high.

The lattice of interest in [27] requires us to define the following generalisation of the square lattice.

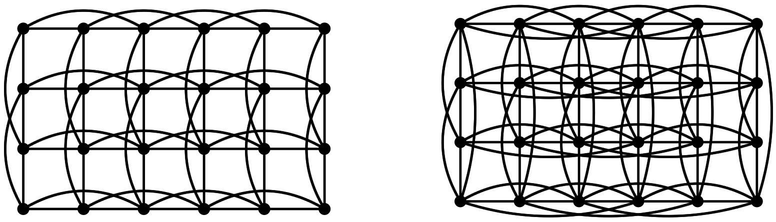


Figure 4.1: Sections of the extended integer lattice as investigated in [27]. The left diagram illustrates $\mathcal{L}_2^2(6,4)$ and the right $\mathcal{L}_3^2(6,4)$, see Definition 4.1.1. Note that we have drawn some edges as curves for visibility but all edges would be straight lines when embedded.

Definition 4.1.1 (ℓ-lattice in d-dimensions, $\mathcal{L}_\ell^d$, (toroidal) $\underline{k}$-section of ℓ-lattice, $\mathcal{L}_\ell^d(\underline{k})$ ($\mathcal{T}_\ell^d(\underline{k})$))**.** *Define $\mathcal{L}_\ell^d$, the ℓ-lattice in d dimensions, to be the graph embedded in $\mathbb{R}^d$ whose vertex set is $\mathbb{Z}^d$ and whose edge set is all axis aligned edges of length at most ℓ.*

For $\underline{k} = (k_1, \ldots, k_n) \in \mathbb{N}^d$ define $\mathcal{L}_\ell(\underline{k})$, the $\underline{k}$-section of $\mathcal{L}_\ell^d$, to be the induced subgraph of $\mathcal{L}_\ell^d$ on vertex set $[k_1] \times \cdots \times [k_d]$.

For $\underline{k}$ as above define $\mathcal{T}_\ell(\underline{k})$, the toroidal $\underline{k}$-section of $\mathcal{L}_\ell^d$, to be the graph embedded in $\mathbb{R}^d$ whose vertex set is $[k_1] \times \cdots \times [k_d]$ and whose edge set is all axis aligned edges with length in $[\ell]$ where edge lengths in the direction of the x_i-axis are considered modulo k_i.

Note that $\mathcal{L}_\ell^d(\underline{k})$ is the embedding of $\prod_i^d P_{k_i}^\ell$ and likewise $\mathcal{T}_\ell^d(\underline{k})$ is the embedding of $\prod_i^d C_{k_i}^\ell$. For the definitions of C_k^ℓ, P_k^ℓ and cartesian products of graphs, see p26. In this chapter we will write $\mathcal{L}_\ell^d(\underline{k})$ and $\mathcal{T}_\ell^d(\underline{k})$ for both the embedded graph and the graph itself.

We can now discuss the paper of Guimerà et al. [27]. In it they give an explicit expression for the modularity of the induced subgraph on a complete rectangular section of $\mathcal{L}_\ell^d$. However, the proof is deferred to a later paper which does not seem to have appeared so for now we call it a conjecture. It is given below in (4.1). We note that they do give a construction for the case of $d = 1$ and $\ell = 1$ which confirms the expression as a lower bound for $\mathcal{L}_1^1$, i.e. a path. Their construction also gives the right order of magnitude for any fixed dimension d and $\ell = 1$ (we have not checked constants) see Lemma 4.1.1.

Lemma 4.1.1 (Guimerà et al. [27]). *Let $d, k, \ell \in \mathbb{N}$ and let $\underline{k} = (k, \ldots, k)$. Then, writing $n = k^d$ for the number of vertices,*

$$q^*(\mathcal{L}^d_\ell(\underline{k})) = 1 - O(n^{-\frac{1}{d+1}}).$$

Indeed it was claimed that for $d, \ell \in \mathbb{N}$ and $\underline{k} = (k_1, \ldots, k_d) \in \mathbb{N}^d$ where $n = \prod_i k_i$,

$$q^*(\mathcal{L}^d_\ell(\underline{k})) = 1 - (d+1)\left(\frac{\ell+1}{2d}\right)^{\frac{d}{d+1}} n^{-\frac{1}{d+1}}. \tag{4.1}$$

For constant d and ℓ, the average degree of a vertex in $\mathcal{L}^d_\ell$ is approximately $2d\ell$ and so equation (4.1) could equivalently be stated in terms of the number of edges m,

$$q^*(\mathcal{L}^d_\ell(\underline{k})) = 1 - (d+1)\left(\frac{\ell(\ell+1)^d}{2^d d^{d-1}}\right)^{\frac{1}{d+1}} m^{-\frac{1}{d+1}}. \tag{4.2}$$

Observe that for constant d, ℓ, equation (4.2) is asymptotically (as $m \to \infty$)

$$q^*(\mathcal{L}^d_\ell(\underline{k})) = 1 - \Theta(m^{-\frac{1}{d+1}}). \tag{4.3}$$

We show in Theorem 4.2.1, for constant ℓ, (4.3) holds as lower bound for the modularity of any m-edge subgraph $\mathcal{R} \subseteq \mathcal{L}^d_\ell$. In Theorem 4.3.1 we show more generally that if a graph can be embedded in $\mathbb{R}^d$ with certain properties this also guarantees modularity $1 - O(m^{-\frac{1}{d+1}})$.

The outline of the chapter is as follows. Lemma 4.2.2 will be central to the proofs of Theorem 4.2.1 and Theorem 4.3.1. In Section 4.2 we state and prove Lemma 4.2.2 and Theorem 4.2.1 follows almost directly. In Section 4.3 we develop some more properties of graph embeddings and end with a proof of Theorem 4.3.1. Lastly we get some upper bounds for the modularity of a particular lattice, $\mathcal{T}^d_1(\underline{k})$. These asymptotically match our lower bounds on $q^*(\mathcal{L}^d_1(\underline{k}))$ from Theorem 4.2.1 and so we can determine the approximate modularity of $\mathcal{T}^d_1(\underline{k})$ and $\mathcal{L}^d_1(\underline{k})$ in Theorem 4.4.1.

In our conference paper [47] we gave the statement of Theorem 4.2.1. Here we provide a proof and a generalisation: Theorem 4.3.1.

4.2 Subgraphs of lattices

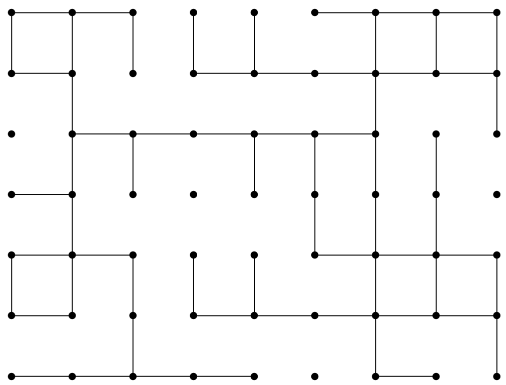


Figure 4.2: A subgraph of the lattice $\mathcal{L}_1^2$. An example of a graph covered by our Theorem 4.2.1 but not by Lemma 4.1.1 of Guimerà et al.

In this section we prove any subgraph of $\mathcal{L}_\ell^d$ with enough edges has high modularity. This forms Theorem 4.2.1. For constant ℓ, the first part of Theorem 4.2.1 extends Lemma 4.1.1 and confirms the claim (4.1) up to order of magnitude in m.

Theorem 4.2.1. *Let $\mathcal{R}$ be an m-edge subgraph of $\mathcal{L}_\ell^d$. Then for $m \geq \ell^{d+1}d^2$,*

$$q^*(\mathcal{R}) \geq 1 - \ell d^{\frac{1}{d+1}} m^{-\frac{1}{d+1}} \left(d^{\frac{1}{d+1}} + d^{-\frac{d}{d+1}} \right),$$

and for $m \geq \ell^{d+1}d$,

$$q^*(\mathcal{R}) \geq 1 - 2\sqrt[5]{4}\ell m^{-\frac{1}{d+1}}.$$

Theorem 4.2.1 is proven on p78. To prove this theorem and also Theorem 4.3.1 in the next section, we rely on Lemma 4.2.2. To state and prove Lemma 4.2.2 we introduce notation for graph embeddings.

Let G be a graph and $\alpha : V(G) \to \mathbb{R}^d$ an embedding which injectively maps the vertices of G into $\mathbb{R}^d$. The map α induces an embedding of the edges: we embed the edge vw to the straight line between $\alpha(v)$ and $\alpha(w)$ and denote it $\alpha(vw)$. Note that the embeddings of two edges need not be disjoint. The Euclidean distance between $\alpha(v)$ and $\alpha(w)$ is denoted $\|\alpha(v) - \alpha(w)\|$.

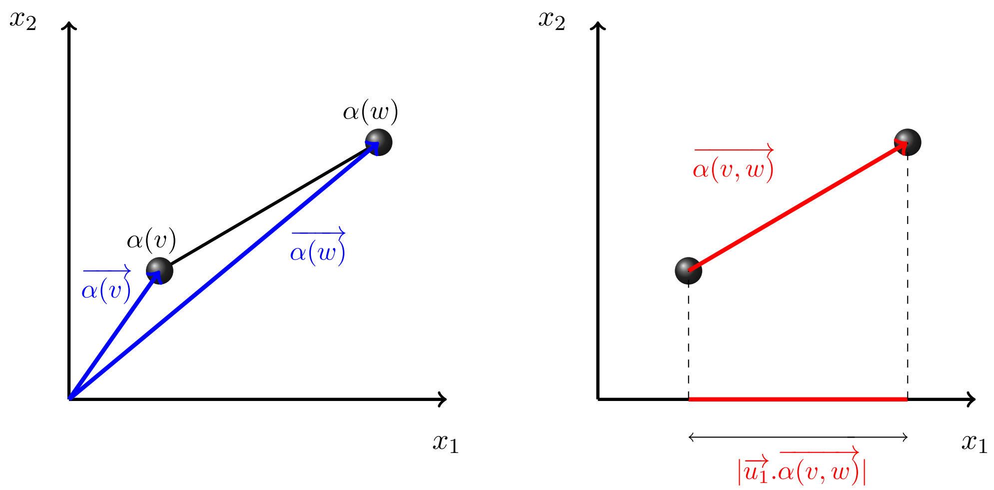


Figure 4.3: We depict the vector from the point $\alpha(v)$ to $\alpha(w)$ in $\mathbb{R}^2$, the embedding α of edge vw and its projection onto the x_1-axis.

Let $\overrightarrow{u_i}$ be the unit vector in the direction of the x_i-axis in $\mathbb{R}^d$. We write $\overrightarrow{\alpha(v)}$ for the vector from the origin to the point $\alpha(v)$. The vector for the embedding of the edge vw (from v to w) is $\overrightarrow{\alpha(v)} - \overrightarrow{\alpha(w)}$ which we denote $\overrightarrow{\alpha(v,w)}$. The absolute value of the dot product $|\overrightarrow{u_1}.\overrightarrow{\alpha(v,w)}|$ gives the length of the embedded edge when projected onto the x_1-axis. See Figure 4.3. Note when calculating this length the absolute value allows us to take $\overrightarrow{\alpha(v,w)}$ or $\overrightarrow{\alpha(w,v)}$ arbitrarily.

We write $\mathbf{C}_\zeta^d$ for a d-dimensional hypercube of side-length ζ and $\mathrm{ds}^* = \mathrm{ds}^*(G,\alpha,\zeta)$ for the maximal degree sum of the embedded graph $\alpha(G)$ in any hypercube $\mathbf{C}_\zeta^d$.

Lemma 4.2.2. *Let G be a graph with m edges. Suppose there is an embedding $\alpha : V(G) \to \mathbb{R}^d$ of G such that, $\forall uv \in E(G)$, $\|\alpha(u) - \alpha(v)\| \le \ell$. Then for $\zeta \ge \ell$,*

$$q^*(G) \ge 1 - \frac{\sqrt{d}\ell}{\zeta} - \frac{\mathrm{ds}^*(G,\alpha,\zeta)}{2m}.$$

Furthermore, if all edges are axis-aligned then,

$$q^*(G) \ge 1 - \frac{\ell}{\zeta} - \frac{\mathrm{ds}^*(G,\alpha,\zeta)}{2m}.$$

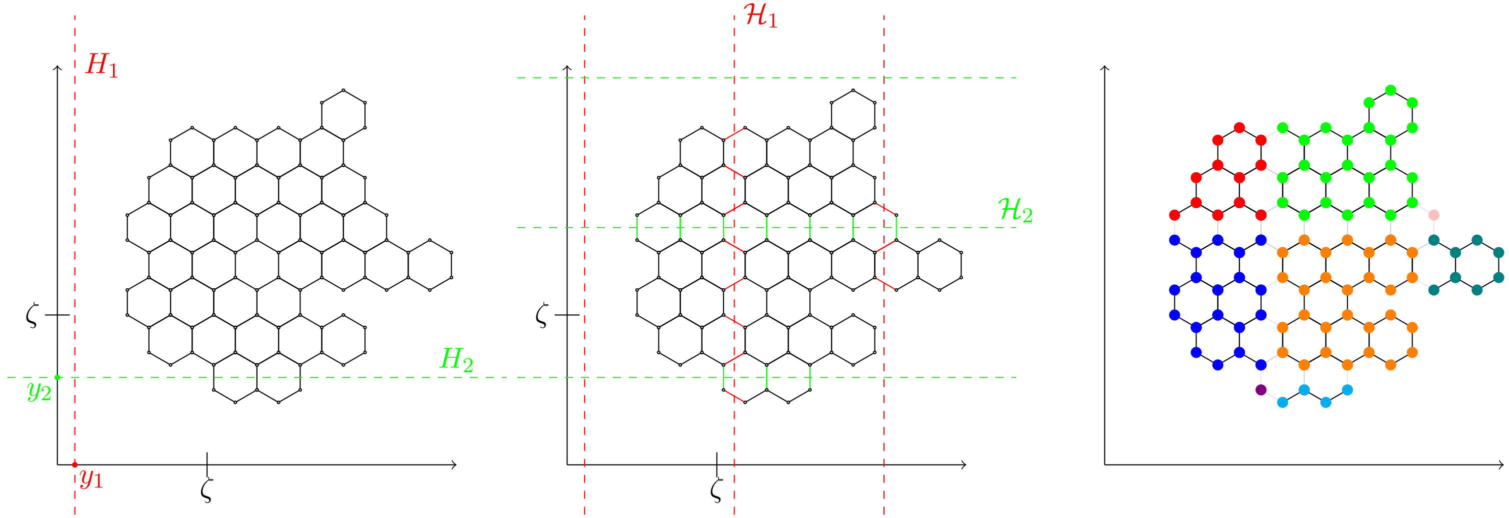


Figure 4.4: Illustration of the grid of hyperplanes used to construct a vertex partition of our embedded graph in Lemma 4.2.2.

Proof. We will split $\mathbb{R}^d$ into boxes using hyperplanes and then use these boxes to define a vertex partition. Figure 4.4 illustrates this construction. Briefly note that if we let V_0 be the set of isolated vertices in G then $q^*(G) = q^*(G \backslash V_0)$ by Lemma 1.4.8 so we may assume that G has no isolated vertices.

Place a hyperplane H_1 perpendicular to the x_1-axis with x_1 co-ordinate, y_1 say, chosen uniformly at random in the interval $[0, \zeta)$. Also place hyperplanes parallel to H_1 at all distances which are a mulitple of ζ and call this set $\mathcal{H}_1 = \mathcal{H}_1(y_1, \zeta)$. The probability that $\mathcal{H}_1$ intersects the embedding of an edge $vw \in E(G)$ is the length of $\alpha(v, w)$ projected onto the x_1-axis divided by the distance between hyperplanes ζ.

$$\mathbb{P}(\alpha(vw) \cap \mathcal{H}_1 \neq \varnothing) = \frac{|\overrightarrow{u_1}.\overrightarrow{\alpha(v,w)}|}{\zeta}$$

Let F_1 be the set of edges which intersect $\mathcal{H}_1$. Then

$$\mathbb{E}(|F_1|) = \frac{1}{\zeta} \sum_{vw \in E(G)} |\overrightarrow{u_1}.\overrightarrow{\alpha(v,w)}|. \tag{4.4}$$

By the first moment method, there exists a z_1 and set of hyperplanes $\mathcal{H}_1(z_1, \zeta)$, denote it $\mathcal{H}_1'$ which intersects at most the number of embedded edges in (4.4).

Similarly, for each $i = 2, \ldots, d$ choose $z_i \in [0, \zeta)$ so that the set of hyperplanes $\mathcal{H}_i' = \mathcal{H}_i(z_i, \zeta)$ intersects the set of edges F_i, and $|F_i|$ is at most the expected number of edges intersected by the random set of hyperplanes $\mathcal{H}_i(y_i, \zeta)$ for $y_i \in_u [0, \zeta)$.

The sets of hyperplanes $\mathcal{H}_1', \ldots, \mathcal{H}_d'$ form an infinite grid in $\mathbb{R}^d$ which we denote $\mathcal{H}$ (illustrated in the first two diagrams in Figure 4.4).

Now we can bound the size of $F = \cup_i F_i$ the set of edges $\mathcal{H}$ intersects. The maximum length of an embedded edge is bounded above by ℓ and so:

$$|F| \leq \sum_{i=1}^{d} |F_i| \leq \tfrac{1}{\zeta} \sum_{i=1}^{d} \sum_{vw \in E(G)} |\overrightarrow{u_i}.\overrightarrow{\alpha(v,w)}| \leq \tfrac{1}{\zeta}\sqrt{d}\ell m. \tag{4.5}$$

We use $\mathcal{H}$ to construct a vertex partition of G in the following way. Label each non-empty box in $\mathcal{H}$ (i.e. each box which contains vertices of G) by $S_1, \ldots, S_k$. The boxes S_i induces a vertex partition $\mathcal{A}_{\mathcal{H}} = \{A_1, \ldots, A_k\}$ where A_i is defined as the set of vertices v whose embedding $\alpha(v)$ lies within the box S_i. (For an example see Figure 4.4.)

Observe that the set of edges between the parts in $\mathcal{A}_{\mathcal{H}}$ is exactly F: the set of edges whose embedding intersects the grid $\mathcal{H}$. Thus we have a lower bound for the edge contribution by (4.5),

$$q^E_{\mathcal{A}_{\mathcal{H}}}(G) \geq 1 - \tfrac{1}{\zeta}\sqrt{d}\ell. \tag{4.6}$$

Recall $\mathrm{ds}^* = \mathrm{ds}^*(G, \alpha, \zeta)$ is the maximum degree sum of $\alpha(G)$ in any d-dim hypercube of side-length ζ. By Lemma 1.6.8 the total degree tax is maximised in the case where each part has this maximal degree sum. Hence

$$q^D_{\mathcal{A}_{\mathcal{H}}}(G) \leq \frac{\mathrm{ds}^*}{2m}. \tag{4.7}$$

The general result now follows by (4.6) and (4.7) as by the definition of modularity $q^*(G) \leq q^E_{\mathcal{A}_{\mathcal{H}}}(G) - q^D_{\mathcal{A}_{\mathcal{H}}}(G)$. For the special case of axis-aligned edges the bound in (4.5) is decreased by a factor of $\sqrt{d}$ which means the lower bound for edge contribution in (4.6) becomes $q^E_{\mathcal{A}_{\mathcal{H}}} \geq 1 - \ell/\zeta$ giving the desired result. □

Now we have established Lemma 4.2.2 the proof of Theorem 4.2.1 will be quick. Before we present that proof we briefly pause to show a simple proposition for the second part of Theorem 4.2.1.

Proposition 4.2.3. *For $d \in \mathbb{N}$, $d^{\frac{1}{d+1}} \leq \sqrt[5]{4}$.*

Proof. Proceed by induction. Notice for $d = 1, 2, 3$ it holds as $1 \leq 4^{\frac{1}{5}}$, $2^{\frac{1}{3}} \leq 4^{\frac{1}{5}}$ and $3 \leq 4^{\frac{1}{5}}$. Now assume true for some $k \geq 4$: assume $k \leq 4^{\frac{k+1}{5}}$. But, for $k \geq 4$, $1 + 1/k \leq 1 + 1/4 \leq 4^{\frac{1}{5}}$ and so we have $k + 1 = k(1 + 1/k) \leq 4^{\frac{k+1}{5}} 4^{\frac{1}{5}} = 4^{\frac{k+2}{5}}$ to complete the induction. □

We can now prove that any subgraph of $\mathcal{L}^d_\ell$ with enough edges has high modularity.

Proof. (of Theorem 4.2.1) First note $\mathcal{L}^d_\ell$ has only axis aligned edges and maximum edge length ℓ. Now we simply observe that for any ζ, $\mathrm{ds}^* \leq 2d\ell(\zeta+1)^d$. Hence if $\mathcal{R}$ is an m-edge subgraph of $\mathcal{L}^d_\ell$ then by Lemma 4.2.2 for $\zeta \geq \ell$, we obtain

$$q^*(\mathcal{R}) \geq 1 - \frac{\ell}{\zeta} - \frac{d\ell(\zeta+1)^d}{m}.$$

If $m \geq \ell^{d+1}d^2$ we can set $\zeta^{d+1} = \frac{m}{d^2}$ to complete the proof of the first part of Theorem 4.2.1. Similarly, for $m \geq \ell^{d+1}d$, we can set $\zeta^{d+1} = \frac{m}{d}$ to get $q^*(\mathcal{R}) \geq 1 - 2d^{\frac{1}{d+1}}m^{-\frac{1}{d+1}}$. Then by Proposition 4.2.3, $d^{\frac{1}{d+1}} \leq \sqrt[5]{4}$, which completes the proof of the second part of the theorem. □

4.3 Graphs which embed with small distortion.

We now extend our result from subgraphs of lattices to graphs which can be embedded with certain properties. At first one might hope to generalise to show high modularity for any graph which embeds with bounded ratio of maximum and minimum edge length. However, for example, a star with n edges, i.e. $K_{1,n}$, has modularity 0 but can be embedded into $\mathbb{R}^2$ so that all edges have equal length. Intuitively the problem is that bounding the ratio between maximum and minimum edge length does not bound the maximum degree. However, it is sufficient to bound a related quantity. We consider the maximum edge length of the embedding but now insist that all vertices are at least unit distance apart. (This is equivalent to bounding the ratio between the maximum edge length and minimum vertex separation.) In Lemma 4.3.4 we show that bounding this ratio leads to a bound on the maximum degree.

In Theorem 4.3.1 we give a lower bound for modularity for any graph which can be embedded into $\mathbb{R}^d$ in terms of the length of the longest embedded edge for embeddings where all vertices are at least unit distance apart.

Theorem 4.3.1. *Let G be a graph with m edges. Suppose there is an embedding $\alpha : V(G) \to \mathbb{R}^d$ of G such that*

$$\forall x \neq y \in V(G),\ \ 1 \leq \|\alpha(x) - \alpha(y)\| \quad \textit{and} \quad \forall uv \in E(G),\ \ \|\alpha(u) - \alpha(v)\| \leq \ell.$$

Then if $m \geq 4^d \ell^{2d} d^{d+2}$,

$$q^*(G) \geq 1 - 7d \left(\frac{\ell^{2d}}{m}\right)^{\frac{1}{d+1}},$$

and for $\ell = 1$, if $m \geq 2d^{\frac{d+2}{2}}$,

$$q^*(G) \geq 1 - 3(1 + \varepsilon_d) d m^{-\frac{1}{d+1}},$$

where $\varepsilon_d \to 0$ as $d \to \infty$.

Distortion is a measure of how much the distance between two points can vary depending on the metric used. In our case one metric is the euclidean distance between the embedded vertices and the other is the graph distance. This has been used before to study the embeddings of certain graphs, see for example [40].

For a graph G we the graph distance d_G is a metric on its vertex set. Define $d_G(x, x) = 0$. For distinct vertices x and y in the same component define $d_G(x, y)$ to be the number of edges in the shortest path between them. If x and y are in different components define $d_G(x, y) = \infty$.

Definition 4.3.1 (distortion)**.** *An embedding α of a graph G into $\mathbb{R}^d$ is said to have* distortion *at most ℓ if for all distinct vertices x, y in the same connected component,*

$$d_G(x, y) \leq \|\alpha(x) - \alpha(y)\| \leq \ell d_G(x, y).$$

Theorem 4.3.1 shows that small distortion also implies high modularity.

Corollary 4.3.2. *Let G be a graph with m edges. Suppose G has an embedding into $\mathbb{R}^d$ with distortion at most ℓ. Then if $m \geq 4^d \ell^{2d} d^{d+2}$,*

$$q^*(G) \geq 1 - 7d \left(\frac{\ell^{2d}}{m} \right)^{\frac{1}{d+1}}.$$

Proof. It suffices to show that distortion ℓ implies there exists an embedding $\alpha : V(G) \to \mathbb{R}^d$ satisfying the conditions of Theorem 4.3.1.

If G has more than one connected component, then we can embed the components far from each other so it suffices to assume G is connected. Fix an embedding α which embeds G with distortion ℓ.

By the definition of distortion, any two vertices u, v in the same connected component have graph distance $1 \leq d_G(u, v)$ and so are also at least unit distance apart in our embedding. It only remains to show that the length of any embedded edge is at most ℓ. However, this follows because if xy is an edge this implies that there is graph distance of one between x and y and so $\|\alpha(x) - \alpha(y)\| \leq \ell d_G(x, y) = \ell$. □

The rest of this chapter is now devoted to developing the proof of Theorem 4.3.1. We will need a few preliminary lemmas, then use these to bound the maximum degree of our graph in Lemma 4.3.4 which will in turn help us bound the maximal degree sum inside a hypercube of a certain size in Lemma 4.3.5.

Definition 4.3.2 (unit packing)**.** *For $X \subset \mathbb{R}^d$ define $U(X)$ to be the maximum number of non-overlapping open balls of unit diameter each of whose centres lies within the closure of X.*

In the special case where the minimum vertex separation and the maximum edge length are both one, we can obtain better bounds on the maximum degree by considering something known as the kissing number, see [11] for a survey.

Definition 4.3.3 (kissing number)**.** *Let the kissing number in d-dimensions, $k(d)$, be the highest number of non-overlapping spheres that can touch a sphere of the same size.*

We will use an upper bound from [32] (as attributed by [11], the paper [32] is in Russian).

Lemma 4.3.3 (Kabatiansky and Levenshtein [32])**.**

$$k(d) \leq 2^{0.401d(1+o(1))}$$

We are now ready to prove upper bounds on the maximum degree of G.

Lemma 4.3.4. *Let G be a graph with m edges. Suppose there is an embedding $\alpha : V(G) \to \mathbb{R}^d$ of G such that*

$$\forall x \neq y \in V(G),\ \ 1 \leq \|\alpha(x) - \alpha(y)\| \quad \textit{and} \quad \forall uv \in E(G),\ \ \|\alpha(u) - \alpha(v)\| \leq \ell.$$

Then

$$\Delta(G) \leq 2^d(\ell + 1/2)^d. \tag{4.8}$$

Proof. Fix $u \in V(G)$. Construct a set $\mathscr{B}$ of open balls with radius a half about the embeddings of each neighbour of u and about u itself (see Figure 4.5 for an example):

$$\mathscr{B} = \{\mathbf{B}_{1/2}(\alpha(v))^d \ : \ v \in \overline{\Gamma}(u)\}.$$

All centres are at least unit distance apart and the open balls around them will not intersect: $\forall$ distinct $v, w \in \Gamma(u)$, $\mathbf{B}_{1/2}(\alpha(v))^d \cap \mathbf{B}_{1/2}(\alpha(w))^d = \varnothing$. Also note each ball in $\mathscr{B}$ has its centre within the closure of $\mathbf{B}_\ell(\alpha(u))^d$. Now, $\deg(u) + 1 = |\overline{\Gamma}(u)| = |\mathscr{B}| \leq U(\mathbf{B}^d_\ell)$.

To prove (4.8) it is sufficient to show $U(\mathbf{B}^d_\ell) \leq 2^d(\ell + 1/2)^d$. Note the maximum number of vertices in $\mathbf{B}^d_\ell$ must be at most the number of spheres of unit diameter that can pack into the closure of $\mathbf{B}^d_{\ell+1/2}$. Thus, $U(\mathbf{B}^d_\ell)\mathrm{vol}(\mathbf{B}^d_{1/2}) \leq \mathrm{vol}(\mathbf{B}^d_{\ell+1/2})$ and $U(\mathbf{B}^d_\ell) \leq 2^d(\ell + 1/2)^d$ as required.

□

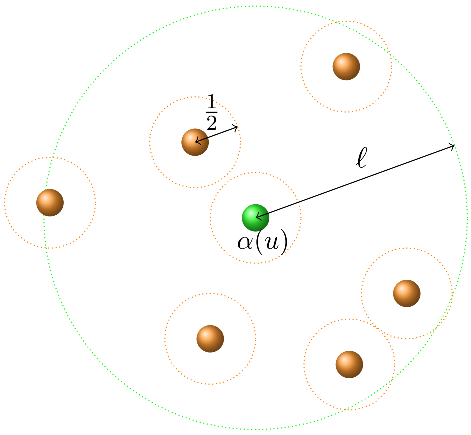


Figure 4.5: Suppose any neighbour of u must embed within distance ℓ of $\alpha(u)$ and the embeddings of all vertices must be at least unit distance apart. This bounds the maximum degree, see Lemma 4.3.4.

Lemma 4.3.5. *Let G be a graph with m edges. Suppose there is an embedding $\alpha : V(G) \to \mathbb{R}^d$ of G such that*

$$\forall x \neq y \in V(G),\ \ 1 \leq \|\alpha(x) - \alpha(y)\| \quad \textit{and} \quad \forall uv \in E(G),\ \ \|\alpha(u) - \alpha(v)\| \leq \ell.$$

Then

$$\mathrm{ds}^*(G, \alpha, \zeta) \leq \frac{2^{\frac{3d-2}{2}} e^{\frac{d}{2\ell} + \frac{d}{\zeta}}}{(\pi e)^{\frac{d-1}{2}}} \ell^d d^{\frac{d+3}{2}} \zeta^d,$$

and for $\ell = 1$

$$\mathrm{ds}^*(G, \alpha, \zeta) \leq \frac{2^{0.901d(1+\varepsilon_d)} e^{\frac{d}{\zeta}}}{2\pi^{\frac{d-1}{2}} e^{\frac{d-1}{2}}} d^{\frac{d+3}{2}} \zeta^d,$$

where $\varepsilon_d \to 0$ as $d \to \infty$.

For the proof of this lemma we will use an approximation for the gamma function which appeared as Theorem 1.5 in [3].

Lemma 4.3.6 (Batir [3]). *For any positive real number x the following holds*

$$\sqrt{2e}\left(\frac{x+1/2}{e}\right)^{x+1/2} \leq \Gamma(x+1) < \sqrt{2\pi}\left(\frac{x+1/2}{e}\right)^{x+1/2}.$$

Proof. (of Lemma 4.3.5) As in the proof of Lemma 4.3.4, $U(\mathbf{C}^d_\zeta)\mathrm{vol}(\mathbf{B}^d_{1/2}) \leq \mathrm{vol}(\mathbf{C}^d_{\zeta+1})$ and hence $U(\mathbf{C}^d_\zeta) \leq 2^d(\zeta+1)^d/\mathrm{vol}(\mathbf{B}^d_1)$. Recall that the volume of a unit sphere in d-dimensions is given by the following formula:

$$\mathrm{vol}(\mathbf{B}_1^d) = \frac{2\pi^{d/2}}{d\Gamma(\frac{d}{2})}.$$

Here the calculations get a little messy. We use the bound on the Gamma function given in Lemma 4.3.6 to deduce a lower bound for the volume of $\mathbf{B}_1^d$.

$$\mathrm{vol}(\mathbf{B}_1^d) \geq \frac{2\pi^{d/2}}{d}\frac{1}{\sqrt{2\pi}}\left(\frac{2e}{d+1}\right)^{\frac{d+1}{2}} = \frac{2^{\frac{d+2}{2}}\pi^{\frac{d-1}{2}}e^{\frac{d+1}{2}}}{d(d+1)^{\frac{d+1}{2}}}.$$

We now have an upper bound for $U(\mathbf{C}_\zeta^d)$:

$$U(\mathbf{C}_\zeta^d) \leq \frac{2^d(\zeta+1)^d}{\mathrm{vol}(\mathbf{B}_1^d)} \leq \frac{2^{\frac{d-2}{2}}}{\pi^{\frac{d-1}{2}}e^{\frac{d+1}{2}}}d(d+1)^{\frac{d+1}{2}}(\zeta+1)^d \leq \frac{2^{\frac{d-2}{2}}d^{\frac{d+3}{2}}e^{\frac{d}{\zeta}}\zeta^d}{\pi^{\frac{d-1}{2}}e^{\frac{d-1}{2}}}. \tag{4.9}$$

where the second inequality follows after a little algebra: $(d+1)^{\frac{d+1}{2}} \leq d^{\frac{d+1}{2}}e^{\frac{1}{2}+\frac{1}{2d}} \leq d^{\frac{d+1}{2}}e$ and $(\zeta+1)^d \leq \zeta^d e^{\frac{d}{\zeta}}$. Finally we are able to bound ds^* by noting it can be at most $\Delta(G)U(\mathbf{C}_\zeta^d)$ and that both terms of this product are bounded in Lemma 4.3.4 and line (4.9) respectively:

$$\mathrm{ds}^* \leq \frac{2^{\frac{3d}{2}}}{2\pi^{\frac{d-1}{2}}e^{\frac{d-1}{2}}}(\ell+1/2)^d\zeta^d e^{\frac{d}{\zeta}}d^{\frac{d+3}{2}} \leq \frac{2^{\frac{3d-2}{2}}e^{\frac{d}{2\ell}+\frac{d}{\zeta}}}{(\pi e)^{\frac{d-1}{2}}}\ell^d d^{\frac{d+3}{2}}\zeta^d$$

where we simplify similarly to above: $(\ell+1/2)^d \leq \ell^d(1+(2\ell)^{-1})^d \leq \ell^d e^{\frac{d}{2\ell}}$. This completes the first part of the theorem and we can move to the case $\ell = 1$.

Fix a vertex v. As $\ell = 1$ any neighbour $u \in \Gamma(v)$ must be embedded at precisely unit distance from $\alpha(v)$. Construct the set of unit diameter open balls around the embeddings of all neighbours of v. These balls are all tangent to $\mathbf{B}_{1/2}(\alpha(v))^d$ and also pairwise do not intersect. Thus the number of such balls is at most the kissing number in d-dimensions (see Definition 4.3.3) and $\Delta(G) \leq k(d)$. By Lemma 4.3.3 and our bound on $U(\mathbf{C}_\zeta^d)$ in (4.9):

$$\mathrm{ds}^* \leq \frac{2^{0.901d(1+\varepsilon_d)}e^{\frac{d}{\zeta}}}{2\pi^{\frac{d-1}{2}}e^{\frac{d-1}{2}}}d^{\frac{d+3}{2}}\zeta^d,$$

where $\varepsilon_d \to 0$ as $d \to \infty$. □

We are now ready to prove the main theorem of this section.

Proof. (of Theorem 4.3.1) We will actually show

$$q^*(G) \geq 1 - 4de^{\frac{1}{\ell}}\sqrt{\frac{2d^{\frac{1}{d+1}}}{\pi e}}\left(\frac{\pi e l^{2d}}{8\sqrt{2e^{\frac{1}{\ell}}}\ m}\right)^{\frac{1}{d+1}}. \tag{4.10}$$

Note $\ell \geq 1$, so $1 \leq e^{\frac{1}{\ell}} \leq e$. Also by Proposition 4.2.3, $\sqrt{d^{\frac{1}{d+1}}} \leq 2^{1/4}$. We can then observe (4.10) implies the theorem by making the substitutions $4\sqrt{2e}\sqrt[4]{2} \leq 7\sqrt{\pi}$ and $\pi e \leq 8\sqrt{2e^{\frac{1}{\ell}}}$.

Lemma 4.2.2 provides a lower bound for modularity in terms of d, ζ, m and $\mathrm{ds}^*(G,\alpha,\zeta)$. Combine this with our upper bound for $\mathrm{ds}^*(G,\alpha,\zeta)$ in Lemma 4.3.5. For any $\zeta \geq \ell$,

$$q^*(G) \geq 1 - \frac{\sqrt{d}\ell}{\zeta} - \frac{2^{\frac{3d}{2}}e^{\frac{d}{2\ell}+\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}}\ell^d d^{\frac{d+3}{2}}\zeta^d. \tag{4.11}$$

We are free to pick a function for ζ as long as $\zeta \geq \ell$. By the condition on m in the theorem statement setting,

$$\zeta = \frac{\sqrt{\pi e}}{2\ell e^{\frac{1}{\ell}}\sqrt{2d}}\left(\frac{8\ell^2 m\sqrt{2e^{\frac{1}{\ell}}}}{\pi e\sqrt{d}}\right)^{\frac{1}{d+1}}, \tag{4.12}$$

will ensure $\zeta \geq 2\ell\sqrt{d}$. Therefore we have $\zeta \geq \ell$ as required and $e^{\frac{d}{\zeta}} \leq e^{\frac{\sqrt{d}}{2\ell}} \leq e^{\frac{1}{2\ell}}$ which we will use later.

To prove the theorem it will suffice to show for ζ as defined in (4.12) that both negative terms in (4.11) have magnitude at most $2de^{\frac{1}{\ell}}\sqrt{\frac{2}{\pi e}}\left(\frac{\pi e\ell^{2d}\sqrt{d}}{8m\sqrt{2e^{\frac{1}{\ell}}}}\right)^{\frac{1}{d+1}}$. The first is not too messy.

$$\frac{\sqrt{d}\ell}{\zeta} = \frac{2d\ell^2 e^{\frac{1}{\ell}}\sqrt{2}}{\sqrt{\pi e}}\left(\frac{\pi e\sqrt{d}}{8\ell^2 m\sqrt{2e^{\frac{1}{\ell}}}}\right)^{\frac{1}{d+1}} = \frac{2de^{\frac{1}{\ell}}\sqrt{2}}{\sqrt{\pi e}}\left(\frac{\pi e\ell^{2d}\sqrt{d}}{8m\sqrt{2e^{\frac{1}{\ell}}}}\right)^{\frac{1}{d+1}}.$$

Now it only remains to show the second term is also small. We substitute our set value for ζ and cancel:

$$\begin{aligned}\frac{2^{\frac{3d}{2}}e^{\frac{d}{2\ell}+\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}}\ell^d d^{\frac{d+3}{2}}\zeta^d &= \frac{2^{\frac{3d}{2}}e^{\frac{d}{2\ell}+\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}}\ell^d d^{\frac{d+3}{2}}\left(\frac{\sqrt{\pi e}}{2\ell e^{\frac{1}{\ell}}\sqrt{2d}}\right)^d\frac{8\ell^2 m\sqrt{2e^{\frac{1}{\ell}}}}{\pi e\sqrt{d}}\left(\frac{\pi e\sqrt{d}}{8\ell^2 m\sqrt{2e^{\frac{1}{\ell}}}}\right)^{\frac{1}{d+1}} \\ &= \frac{e^{\frac{d}{\zeta}}}{e^{\frac{d}{2\ell}}}\frac{2\ell^2 d\sqrt{2e^{\frac{1}{\ell}}}}{\sqrt{\pi e}}\left(\frac{\pi e\sqrt{d}}{8\ell^2 m\sqrt{2e^{\frac{1}{\ell}}}}\right)^{\frac{1}{d+1}}\end{aligned} \tag{4.13}$$

Now use $e^{\frac{d}{\zeta}} \leq e^{\frac{d}{2\ell}}$ and $\sqrt{e^{\frac{1}{\ell}}} \leq e^{\frac{1}{\ell}}$ to deduce from (4.13):

$$\frac{2^{\frac{3d}{2}} e^{\frac{d}{2\ell}+\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}} \ell^d d^{\frac{d+3}{2}} \zeta^d \quad \leq \quad \frac{2\ell^2 d e^{\frac{1}{\ell}} \sqrt{2}}{\sqrt{\pi e}} \left(\frac{\pi e \sqrt{d}}{8\ell^2 m \sqrt{2e^{\frac{1}{\ell}}}} \right)^{\frac{1}{d+1}},$$

which suffices to prove (4.10). Now we turn our attention to the special case of $\ell = 1$. The method is the same but a better bound for ds* in Lemma 4.3.4 will allow a better lower bound for modularity. By this bound for ds* and Lemma 4.2.2 for $\zeta \geq \ell$,

$$q^*(G) \geq 1 - \frac{\sqrt{d}}{\zeta} - \frac{2^{0.901d(1+\varepsilon_d)} e^{\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}} d^{\frac{d+3}{2}} \zeta^d, \tag{4.14}$$

where $\varepsilon_d \to 0$ as $d \to \infty$. As $m \geq 2d^{\frac{d+2}{2}}$, we can set

$$\zeta = \frac{\sqrt{\pi}}{2^{0.901}\sqrt{d}} \left(\frac{4m}{\pi e \sqrt{d}} \right)^{\frac{1}{d+1}},$$

to ensure $\zeta \geq 2$, which means (4.14) holds and $e^{\frac{d}{\zeta}} \leq \sqrt{e}$. We continue by showing both negative terms in (4.14) are small. By our choice of ζ,

$$\frac{\sqrt{d}}{\zeta} = d \frac{2^{0.901} e^{\frac{1}{d+1}} \sqrt{d}^{\frac{1}{d+1}}}{\sqrt{\pi}} \left(\frac{\pi}{4m} \right)^{\frac{1}{d+1}}.$$

Note that $e^{\frac{1}{d+1}} \leq \sqrt{e}$ and by Proposition 4.2.3, $d^{\frac{1}{2(d+1)}} \leq \sqrt[4]{2}$ which lets us calculate that $\frac{2^{0.901}\sqrt{e}\sqrt[4]{2}}{\sqrt{\pi}} < 2.07$. Hence

$$\frac{\sqrt{d}}{\zeta} \leq 2.1 d m^{-\frac{1}{d+1}}. \tag{4.15}$$

To complete the proof it is now be sufficient to show the other negative term in (4.14) is also small. Again, by our choice of ζ, many terms cancel:

$$\frac{2^{0.901d(1+\varepsilon_d)} e^{\frac{d}{\zeta}}}{4m(\pi e)^{\frac{d-1}{2}}} d^{\frac{d+3}{2}} \zeta^d = \frac{2^{\varepsilon_d} d \sqrt{d}^{\frac{1}{d+1}} e^{\frac{1}{d+1}}}{\sqrt{\pi e}} \left(\frac{\pi}{4m} \right)^{\frac{1}{d+1}} \leq 0.7 \cdot 2^{\varepsilon_d} d m^{-\frac{1}{d+1}}. \tag{4.16}$$

Recall $e^{\frac{1}{d+1}} \leq \sqrt{e}$ and $d^{\frac{1}{2(d+1)}} \leq \sqrt[4]{2}$ and calculate $\sqrt[4]{2}/\sqrt{\pi} \leq 0.7$ to infer the inequality above. Now by (4.16) and (4.15), in the special case $\ell = 1$:

$$q^*(G) \leq 3 \cdot 2^{\varepsilon_d} d m^{-\frac{1}{d+1}},$$

and we are done. $\square$

An interesting corollary of this is that we can determine minimum bounds for the distortion of graphs. For example, a random cubic graph whp has modularity at most 0.81 which implies that the distortion of any embedding in $\mathbb{R}^d$ must be at least $\frac{1}{50d}\left(\frac{m}{d}\right)^{\frac{1}{2d}}$.

4.4 Upper bounds for the Integer Lattice

In this section we restrict our attention to complete sections of the 1-lattice and determine its modularity in Theorem 4.4.1. We do this for both the toroidal and non-toroidal case, see Definition 4.1.1.

This requires proving upper bounds for the modularity. We develop Lemma 4.4.4 which allows us to bound the maximum modularity in terms of a function of the maximum number of internal edges inside vertex subsets of various sizes, the number of vertices in the graph and the number of edges in the graph. This can then be combined with a result of Bollobás and Leader, see Lemma 4.4.3, who studied the maximal number of edges induced by vertex subsets of $\mathcal{L}_1^d$. The resulting upper bounds on the modularityasymptoticly match the lower bounds in Theorem 4.2.1, showing Theorem 4.2.1 is tight in this case and giving us Theorem 4.4.1.

Theorem 4.4.1. *Let* $\underline{k} = (k, k, \ldots, k) \in \mathbb{N}^d$*. Let* $G \in \{\mathcal{T}_1^d(\underline{k}), \mathcal{L}_1^d(\underline{k})\}$ *and write* $m = e(G)$ *for the number of edges. Then for* $d = o(k)$*,*

$$q^*(G) = 1 - \frac{d^{\frac{1}{d+1}}}{m^{\frac{1}{d+1}}} \left(d^{\frac{1}{d+1}} + d^{-\frac{d}{d+1}} \right) (1 + o(1)).$$

Theorem 4.4.2. *Let* $\underline{k} = (k, k, \ldots, k) \in \mathbb{N}^d$*. Let* $G \in \{\mathcal{T}_1^d(\underline{k}), \mathcal{L}_1^d(\underline{k})\}$ *and write* $m = e(G)$ *for the number of edges. Then for* $d = o(k)$*,*

$$1 - \frac{2 + \sqrt{2}}{m^{\frac{1}{d+1}}} \leq q^*(G) \leq 1 - \frac{1}{m^{\frac{1}{d+1}}} (1 + o(1)).$$

Observe that in one dimension the toroidal lattice $\mathcal{T}_1^1(n)$ is simply a cycle on n vertices and n edges. Hence our theorem implies $q^*(C_n) = 1 - 2n^{-1/2}(1 + o(1))$ as earlier proven by Brandes et al. in [13].

Recall that $\mathcal{L}_1^d$ is the infinite integer grid in d dimensions: see Definition 4.1.1 on p72. The proof of this theorem will leverage an isoperimetric result of Bollobás and Leader. They determined for any given number of vertices the maximal number of edges which can be induced by a subset of that size in $\mathcal{L}_1^d$. In particular, we use Corollary 16 in [7] which we repeat below.

Lemma 4.4.3 (Bollobás and Leader [7]). *For $s = 1, \dots, k$, if $A \subset V(\mathcal{L}_1^d)$ with $|A| \le s^d$ then $e(A) \le d(1 - \frac{1}{s})|A|$ with equality when $A = [s]^d$.*

The following lemma will allow us to find an upper bound for modularity in terms of a function of maximal number of internal edges inside a set and the size of that set. We will apply it in the proof of Theorem 4.4.1 with G a toroidal lattice and G' the non-toroidal lattice on same vertex set. This lemma is a generalisation of Lemma 2.3.1 on p59.

Lemma 4.4.4. *Let G be a regular graph with m edges and n vertices. Let $E \subset E(G)$ and write $G' = G \backslash E$. Then*

$$q^*(G) \le \frac{|E|}{m} + \max_{A \subseteq V(G)} \left(\frac{e_{G'}(A) n}{|A| m} - \frac{|A|}{n} \right).$$

Proof. Fix an optimal vertex partition $\mathcal{A} = \{A_1, \dots, A_k\}$ and we can bound the modularity in terms of numbers of internal edges in G'.

$$q_{\mathcal{A}}(G) = \sum_i \frac{e(A_i)}{m} - \frac{|A_i|^2}{n^2} \le \frac{|E|}{m} + \sum_i \frac{e_{G'}(A_i)}{m} - \frac{|A_i|^2}{n^2}$$

Now write $a_i = |A_i|/n$ and rearrange:

$$q_{\mathcal{A}}(G) - \frac{|E|}{m} \le \sum_i a_i \left(\frac{e_{G'}(A_i)}{a_i m} - a_i \right). \tag{4.17}$$

As $\sum_i a_i = 1$, (4.17) allows us to write an upper bound in terms of a single vertex part in $\mathcal{A}$

$$q_{\mathcal{A}}(G) - \frac{|E|}{m} \le \max_i \left(\frac{e_{G'}(A_i)}{a_i m} - a_i \right) \le \max_{A \subseteq V(G)} \left(\frac{e_{G'}(A) n}{|A| m} - \frac{|A|}{n} \right).$$

□

Proof. (of Theorem 4.4.1) We first prove the theorem statement for the toroidal case: $\mathcal{T}_1^d(\underline{k})$. Apply Lemma 4.4.4 with $G = \mathcal{T}_1^d(\underline{k})$ and $G' = \mathcal{L}_1^d(\underline{k})$. The toroidal lattice $\mathcal{T}_1^d(\underline{k})$ is a regular graph of degree $2d$ so $m = e(\mathcal{T}_1^d(\underline{k})) = dn$. For $\mathcal{L}_1^d(\underline{k})$ substitute $A = [k]^d$ into Lemma 4.4.3 to get $e(\mathcal{L}_1^d(\underline{k})) = d(1 - 1/k)n = m(1 - 1/k)$. Write $[k]^d$ for the vertex set and note $\mathcal{L}_1^d\big|_{[k]^d} = \mathcal{L}_1^d(\underline{k})$. By Lemma 4.4.4:

$$q^*(\mathcal{T}_1^d(\underline{k})) \le \frac{1}{k} + \max_{A \subseteq [k]^d} \left(\frac{e_{\mathcal{L}_1^d}(A) n}{|A| m} - \frac{|A|}{n} \right). \tag{4.18}$$

If $(s-1)^d < |A| \leq s^d$ for $s = 2, \ldots, k$, then by Lemma 4.4.3 $e_{\mathcal{L}_1^d}(A) \leq d(1-1/s)|A| = m(1-1/s)|A|/n$ and we can also bound $|A|/n$:

$$\max_{(s-1)^d < |A| \leq s^d} \left(\frac{e_{\mathcal{L}_1^d}(A)n}{|A|m} - \frac{|A|}{n} \right) \leq 1 - \frac{1}{s} - \frac{(s-1)^d}{n} = 1 - \frac{1}{s} - \frac{m(s-1)^d}{d}.$$

We are left with a simple optimisation problem.

$$\max_{A \subseteq [k]^d} \left(\frac{e_{\mathcal{L}_1^d}(A)n}{|A|m} - \frac{|A|}{n} \right) \leq 1 + \min_{s \in \mathbb{R}} \frac{1}{s} + \frac{d(s-1)^d}{m}.$$

By taking derivatives and using the second moment test it follows that the minimum is obtained for s in the range: $m^{\frac{1}{d+1}} d^{-\frac{2}{d+1}} \leq s \leq m^{\frac{1}{d+1}} d^{-\frac{2}{d+1}} + 1$. But $d^2 = o(m)$ so the minimum is $s = m^{\frac{1}{d+1}} d^{-\frac{2}{d+1}}(1+o(1))$. Now substitute this into (4.18), noting that $k^{-1} = n^{-1/d} = d^{1/d} m^{-1/d}$ and $d^{1/d} \leq 2$ which gives $k^{-1} \leq 2m^{-1/d} = o(m^{\frac{1}{d+1}})$.

$$q^*(\mathcal{T}_1^d(\underline{k})) \leq 1 - \frac{d^{\frac{1}{d+1}}}{m^{\frac{1}{d+1}}} \left(d^{\frac{1}{d+1}} + d^{-\frac{d}{d+1}} \right) (1+o(1)). \tag{4.19}$$

We will return to (4.19).

As observed earlier in the proof the graphs $\mathcal{T}_1^d(\underline{k})$ and $\mathcal{L}_1^d(\underline{k})$ have the same vertex set, $E(\mathcal{L}_1^d(\underline{k})) \subset E(\mathcal{T}_1^d(\underline{k}))$ and $|E(\mathcal{T}_1^d(\underline{k})) \backslash E(\mathcal{L}_1^d(\underline{k}))| = m/k$, where $m = e(\mathcal{T}_1^d(\underline{k}))$. Hence by Theorem 1.4.6,

$$|q^*(\mathcal{T}_1^d(\underline{k})) - q^*(\mathcal{L}_1^d(\underline{k}))| \leq \frac{5}{k} = o(m^{\frac{1}{d+1}}). \tag{4.20}$$

The lower bound on $q^*(\mathcal{L}_1^d(\underline{k}))$ in Theorem 4.2.1 together with (4.20) implies a lower bound for $q^*(\mathcal{T}_1^d(\underline{k}))$. As, $m = e(\mathcal{T}_1^d(\underline{k})) = e(\mathcal{L}_1^d(\underline{k}))(1+o(1))$,

$$q^*(\mathcal{T}_1^d(\underline{k})) \geq 1 - \frac{d^{\frac{1}{d+1}}}{m^{\frac{1}{d+1}}} \left(d^{\frac{1}{d+1}} + d^{-\frac{d}{d+1}} \right) (1+o(1)). \tag{4.21}$$

The upper and lower bounds for $q^*(\mathcal{T}_1^d(\underline{k}))$ in (4.19) and (4.21) match and the theorem is proven for the toroidal case $\mathcal{T}_1^d(\underline{k})$. For the non-toroidal case, the lower bound for $q^*(\mathcal{L}_1^d(\underline{k}))$ is given in Theorem 4.2.1 and the upper bound follows from the upper bound for $q^*(\mathcal{T}_1^d(\underline{k}))$ in (4.19), the equation (4.20) and recalling $e(\mathcal{T}_1^d(\underline{k})) = e(\mathcal{L}_1^d(\underline{k}))(1+o(1))$. □

4.5 Further work.

In Theorem 4.4.1 we show lower bounds for the modularity of the 1−lattice are tight. We were able to prove this using isoperimetric bounds on the maximal number of internal edges that can be contained in any n-vertex subset of $\mathcal{L}_1^d$. As part of the proof in [7], Bollobás and Leader give a particular n-vertex subset of $\mathcal{L}_1^d$ for each n such that it contains the maximal number of edges of any n-vertex subset. This is known as the cube order. Interestingly for $\ell > 1$, this cube order no longer gives the maximal construction for each n, see Figure 4.6. This suggests new techniques may be needed to prove similar isoperimetric results to Lemma 4.4.3 for ℓ-lattices where $\ell > 1$.

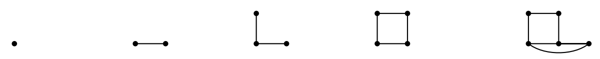
n	1	2	3	4	5
cube order					
edges	0	1	2	4	6
alternate order					
edges	0	1	3	5	7

Figure 4.6: Maximal number of internal edges for 2-lattice in two dimensions.

Chapter 5

Random Regular Graphs

This chapter establishes numerical bounds for the likely maximum modularity of random regular graphs. We use a technique from Chapter 2 to upper bound the modularity via the edge expansion of small vertex sets in the graph.

In applications when a partition is found by approximately optimising modularity over a real network it is important to determine whether the partition found is significant. Thus one would want to define a null model, or probability space, for the network and show that, at the very least, the modularity of the partition found for the data set exceeds the modularity likely in the random instance. This chapter and the next provide the first rigorous upper bounds on the likely maximum modularity of any random graph models.

A preliminary version of these results appeared in [47]. This paper contained the likely lower bound for random cubic graphs via the construction based on Hamiltonian cycles as in Theorem 5.2.1. It also included a likely upper bound for the modularity for random cubic graphs of 0.88 when the maximal size of a part in the partitions was restricted. This result has been superseded by Theorem 5.2.1 which shows a likely upper bound of 0.81 over all possible partitions of the graph.

5.1 Bisection width in random regular graphs.

In this section we review existing results on the likely bisection width of random regular graphs. These will be used to prove likely lower bounds for the maximum modularity of random regular graphs in Theorem 5.2.1, see also Table 5.1.

r	$=$	3	4	5	6	7	8	9	10	11	12
$\frac{1}{n}\mathrm{bw}(G_{n,r})$	$\preceq$	$0.16\dot{6}$	$0.33\dot{3}$	0.503	0.668	0.851	1.039	1.232	1.428	1.624	1.823
$q^*(G_{n,r})$	$>$	0.388	0.333	0.298	0.277	0.256	0.240	0.226	0.214	0.204	0.196

Table 5.1: The likely bounds of both the bisection width of random r-regular graphs from [18,19,49] and of the maximum modularity which were computed using these bisection results in Theorem 5.2.1.

The bisection width parameter has been well studied in random regular graphs. The three papers [18, 19, 49] between them the best published bounds known. The honour is shared, for cubic graphs Monien and Preis [49] derive better bounds while for 4-regular graphs the bounds found by Díaz, Do, Serna and Wormald in [18] are tighter and for $r = 5, \dots, 12$ the bounds are provided by Díaz, Serna and Wormald in [19].

The lower bounds in Theorem 5.2.1 use only the bounds by Díaz, Serna and Wormald for $r = 9, \dots, 12$, as we have a different construction which yields a higher modularity for smaller r. However in Table 5.1 we compile the bisections width for each $r = 3, \dots, 12$ and show the likely lower bound for modularity which it implies. To present these results we use the notation $a \preceq b$ to indicate that $a < b(1 + o(1))$ see Definition 1.2.1 and $\mathrm{bw}(G)$ to indicate the bisection width of graph G as described in Definition 1.5.1.

Lemma 5.1.1 (Monien and Preis [49]). *Let G be any cubic graph on n vertices. Then* $\mathrm{bw}(G) \leq n/6$.

Lemma 5.1.2 (Diaz et al. [18]). *Let $G_{n,4}$ be a random 4-regular graph on n vertices. Then whp* $\mathrm{bw}(G_{n,4}) \preceq n/3$.

The paper by Diaz, Serna and Wormald [19] provide the remaining bounds on the bisection width for r-regular graphs for r up to 12.

Lemma 5.1.3 (Diaz et al. [19]). *Let $G_{n,r}$ be a random r-regular graph on n vertices. Then for $r = 5, \dots, 12$ whp $\mathrm{bw}(G_{n,r})$ satisfies the upper bound in the first line of Table 5.1.*

5.2 Asymptotic modularity for random regular graphs

We can now state our result. As well as the numerical bounds obatined in the theorem, Figure 5.1 and Table 5.2 show simulation data. We denote the results of simulations by $s(G_r^*)$.

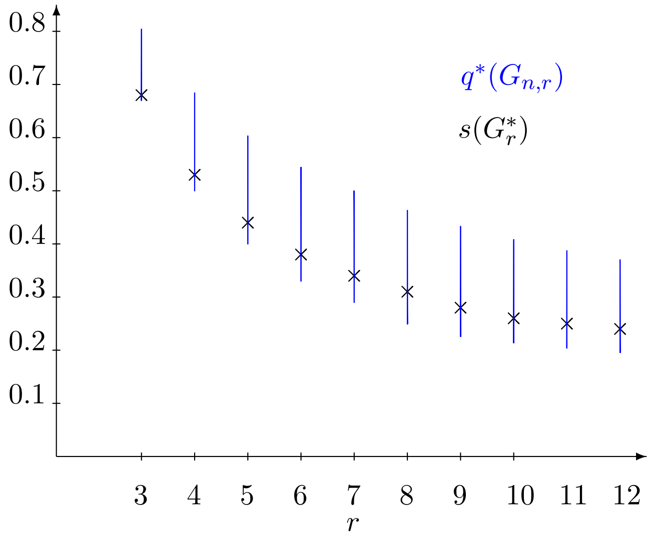


Figure 5.1: Simulation results for $n = 10,000$ nodes and degrees $r = 3, \ldots, 10$. Each cross indicates the maximal computed modularity returned, averaged over ten sampled graphs. The maximum modularity of a random regular graph whp will lie in the interval shown in blue on the same graph, proven in Theorem 5.2.1.

$r =$	3	4	5	6	7	8	9	10	11	12
$q^*(G_{n,r}) >$	0.666	0.500	0.400	0.333	0.285	0.250	0.226	0.214	0.204	0.196
$s(G_r^*) =$	0.68	0.53	0.44	0.38	0.34	0.31	0.28	0.26	0.25	0.24
$q^*(G_{n,r}) <$	0.804	0.684	0.603	0.544	0.499	0.463	0.433	0.408	0.388	0.370

Table 5.2: Modularity of random regular graphs. The first and third rows respectively show the upper and lower bounds for the maximum modularity proven in Theorem 5.2.1. The middle row gives simulation results on randomly generated r-regular graphs with 10000 nodes, modularity estimated using the Louvain method [4].

Graphs G_r^* were generated on 10 000 vertices via the configuration model and rejected if loops or multiple edges occurred. Hence G_r^* would be distributed as a random r-regular graph if our pseudorandom number generator was perfect. The maximum modularity was then estimated by the Louvain method as in [4]. The average over ten runs is shown to two decimal places in the middle row Table 5.2.

Theorem 5.2.1. *Let $G_{n,r}$ be a random r-regular graph on n vertices. For $r = 3, \dots, 12$ the modularity of an r-regular random graph whp lies between the values in the first and third rows of Table 5.2.*

The proof will use results on the u-edge expansion, $i_u(G)$, which were found by Kolesnik and Wormald [35]. Their results imply, for example, that for a random cubic graph $G_{n,r}$ whp $i_{0.2}(G_{n,3}) \succeq 0.32$ and whp $i_{0.01}(G_{n,3}) \succeq 0.57$. To recall the notion of u-edge expansion see Definition 2.2.1 on p57.

Proof. We begin with the upper bounds. Recall that by Corollary 2.2.2 to show any r-regular graph H has modularity less than $1 - \alpha$ it suffices to show that $u + i_u(H)/r > \alpha$ for all $0 < u \leq 1/2$. Detailed results which give a likely upper bound on $i_u(G_{n,r})$ as a function of u were obtained by Kolesnik and Wormald in [35]. They defined a function $f_r(u)$ and proved that whp $i_u(G_{n,r}) > f_r(u)$. Therefore to prove whp $q^*(G) < 1 - \alpha$ it is enough to show $u + f_r(u) > \alpha$ for all $0 < u \leq 1/2$. This implies the upper bounds in Table 5.2.

For the lower bounds we have two techniques. Robinson and Wormald showed that for $r \geq 3$ whp $G_{n,r}$ is Hamiltonian [57, 58]. Hence by Lemma 1.5.2 whp $q^*(G_{n,r}) \geq 2/r + o(1)$ which provides the lower bounds in Table 5.2 for $r = 3, \dots, 8$. For the remaining lower bounds recall that by Lemma 1.5.1, for any r-regular graph H, $q^*(H) \geq 1/2 - 2bw(H)/(rn) + o(1)$. This and the likely bounds for $bw(G_{n,r})$ by Diaz et al. in Lemma 5.1.3 imply the lower bounds for $r = 9, \dots, 12$ in Table 5.2. $\square$

Remark. Our result that a random cubic graphs $G_{n,3}$ whp has modularity at most 0.804 implies via Theorem 3.1.1 that whp $\text{tw}(G_{n,3}) \geq \frac{n}{200}$. It is known a random r-regular graph $G_{n,r}$ whp satisfies $\text{tw}(G_{n,r}) = \Theta(n)$, see [52]. The lower bound for random cubic graphs is not given explicitly in [52] but their results imply $\text{tw}(G_3) \geq n/46 + O(1)$ when coupled with the isoperimetric bounds in [36].

Chapter 6

Erdős-Rényi Random Graphs

This chapter investigates maximum modularity of Erdős-Rényi random graphs.

Three different phases of the likely maximum modularity are found. There is a coarse threshold at $p = 1/n$: for $p \ll 1/n$ (indeed for $np \leq 1 + o(1)$) whp the maximum modularity is near one and for $p \gg 1/n$ whp the maximum modularity is near 0. Inbetween these ranges, when $np \to c$ for constant $c > 1$, we find non-trivial maximum modularity. These statements are made precise in Theorem 6.1.1, with a more detailed breakdown of the likely maximum modularity for different ranges of p in Figure 6.12 on p140.

In Section 6.1 we set the scene, state our results and then give an outline of the chapter on p102.

6.1 Statement of results

6.1.1 Three phases of maximum modularity

In this chapter we study the behaviour of maximum modularity in Erdős-Rényi random graphs which can be broadly summarised in the following theorem. To state the theorem we will use the following shorthand. We say for sequence of random variables $\{X_n\}$, that whp $X_n \to a$, if $\forall \varepsilon > 0$, whp $|X_n - a| < \varepsilon$.

Theorem 6.1.1. *Suppose G_n is a random graph from $\mathcal{G}(n,p)$ for some $p = p(n)$.*
(i) If $n^2p \to \infty$ and $np \leq 1 + o(1)$ then whp

$$q^*(G_n) \to 1.$$

(ii) If $np \to c$ for constant $c > 1$ then $\exists \varepsilon = \varepsilon(c) > 0$ such that whp

$$\varepsilon < q^*(G_n) < 1 - \varepsilon.$$

Furthermore there exist positive functions $a(c),\ b(c)$ with $b(c) \to 0$ as $c \to \infty$, such that whp

$$a(c) < q^*(G_n) < b(c).$$

(iii) If $np \to \infty$ then whp

$$q^*(G_n) \to 0.$$

Theorem 6.1.1 identifies three ranges of edge probability which result in very different modes of behaviour of the maximum modularity of Erdős-Rényi random graphs. This is the main contribution of this chapter. More precise asymptotic results are also proven and we list these along with a brief description of the phase transition in the rest of this introductory section. We defer the proofs of all results until later sections. The proof of Theorem 6.1.1 appears on p138.

6.1.2 Background: appearance of the giant component

A much celebrated phenomenon of random graphs is the phase transition associated with the size of the 'giant' (i.e. largest connected) component in the Erdős-Rényi random graph. Let $L_1(G), L_2(G)$ denote the size (i.e. number of vertices) of the largest and second largest connected components of G.

Lemma 6.1.2 (Erdős and Rényi [22])**.** *Fix $c > 0$ and suppose G_n is a random graph from $\mathcal{G}(n, c/n)$ for some constant c. Then whp*

$$L_1(G_n) = \begin{cases} \Theta(\log n) & \text{if } c < 1 \\ \Theta(n^{2/3}) & \text{if } c = 1 \\ (1 - t/c)n(1 + o(1)) & \text{if } c > 1, \text{ where } t \in (0,1) \text{ solves } te^{-t} = ce^{-c}. \end{cases}$$

and $L_2(G_n) = O(\log n)$ if $c > 1$.

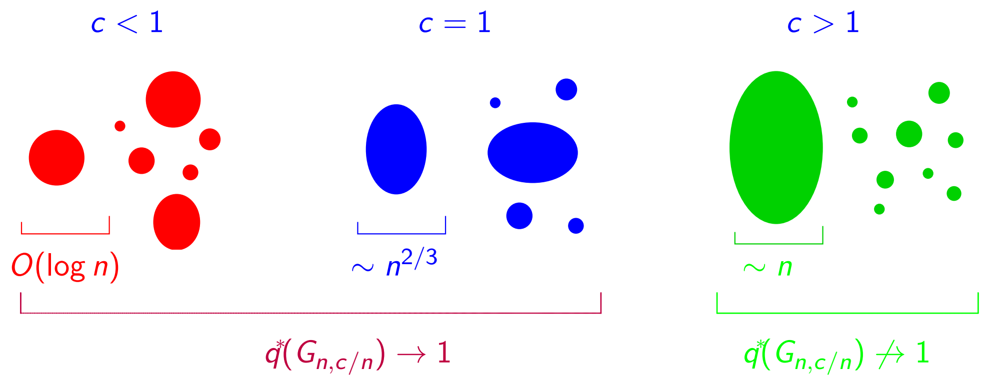


Figure 6.1: An illustration of the likely sizes of connected components in $\mathcal{G}_{n,c/n}$ and showing for which c the likely maximum modularity tends to one. Image credit for the circle illustration: Mihyun Kang, TU Graz, used with permission.

This phenomenon is expressed by saying we have a *phase transition* for the size of the giant component at $p = 1/n$. In this chapter we will show the modularity of $G_{n,p}$ also undergoes a phase transition at this point. As established in Theorem 6.1.1, $q^*(G_{n,c/n}) \to 1$ for $c \leq 1$ but not for $c > 1$.

Much research has been directed into properties of random graphs 'around' $p = 1/n$. The following parametrisation, of $np = 1 + \gamma$, $\gamma = o(1)$ allows a more in depth idea of the structure of the random graph about criticality and is referred to as the critical window.

Lemma 6.1.3 (Bollobás [6], Łuczak [42])**.** *Let $np = 1+\gamma$ for $\gamma = o(1)$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Then whp*

$$L_1(G_n) = \begin{cases} 2\gamma^{-2}(\log(-\gamma^3 n))(1+o(1)) & \text{if } \gamma^3 n \to -\infty \\ \Theta(n^{2/3}) & \text{if } \gamma^3 n \to \lambda \in (-\infty, \infty) \\ 2\gamma n - 5\gamma^2 n/3 + O(\gamma^3 n) & \text{if } \gamma^3 n \to \infty \end{cases}$$

We will study the maximum moduarity of random graphs in the critical window, see Theorem 6.1.4.

6.1.3 Maximum modularity of Erdős-Rényi random graphs

The following result is a more detailed version of Theorem 6.1.1.

Theorem 6.1.4. *Suppose G_n is a random graph from $\mathcal{G}(n,p)$ for some $p = p(n)$. If $n^2p \to \infty$ and $np \leq c + o(1)$ for constant $c < 1$, then whp*

$$q^*(G_n) = 1 - \Theta\left(\frac{1}{n^2p}\right),$$

if $np = 1+\gamma$ for $\gamma = o(1)$, then whp

$$q^*(G_n) = \begin{cases} 1 - O(\frac{1}{\gamma n}) & \text{if } \gamma^3 n \to -\infty \\ 1 - O\left(\frac{1}{n^{2/3}}\right) & \text{if } \gamma^3 n \to \lambda \in (-\infty, \infty) \\ 1 - O(\gamma^3) - O\left(\gamma\sqrt{\frac{\log n}{n \log\log n}}\right) & \text{if } \gamma^3 n \to \infty \end{cases}$$

if $np \to c$ for constant $c > 1$, then whp

$$\frac{1}{c+1} < q^*(G_n) < \max\left\{\frac{32 \log c}{c^{1/3}}, 1\right\}$$

and finally if $np \to \infty$, then whp $q^*(G_n) = o(1)$.

Theorem 6.1.4 is proven on p139.

6.1.4 Structure of an optimal partition

In the lower window an interesting transition takes place. See Figure 6.3 for an illustration.

Theorem 6.1.5. *Define $\gamma^- = \frac{(\log n)^{1/2}}{3n^{1/4}}$ and $\gamma^+ = \frac{(\log n)^{1/4}}{n^{1/4}}$. If $n^2p \to \infty$ and $np \leq 1 - \gamma^-$ then whp the connected components partition is the unique optimal partition. If $np \geq 1 - \gamma^+$ and $np = O(1)$ then whp there is a partition with higher modularity than the connected components partition.*

Note that $\gamma^- > \gamma^+$ and both are $n^{-1/4+o(1)}$. The proof of Theorem 6.1.5 can be found on p123.

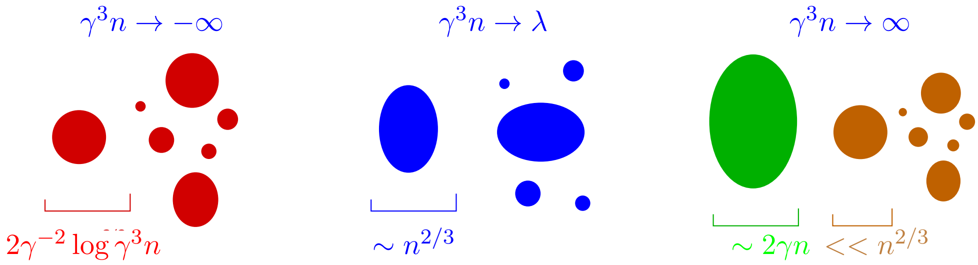


Figure 6.2: An illustration of the likely sizes of connected components in $\mathcal{G}(n,p)$ for $np = 1+\gamma$ and $\gamma = o(1)$. Image credit for the circle illustration: Mihyun Kang, TU Graz, used with permission.

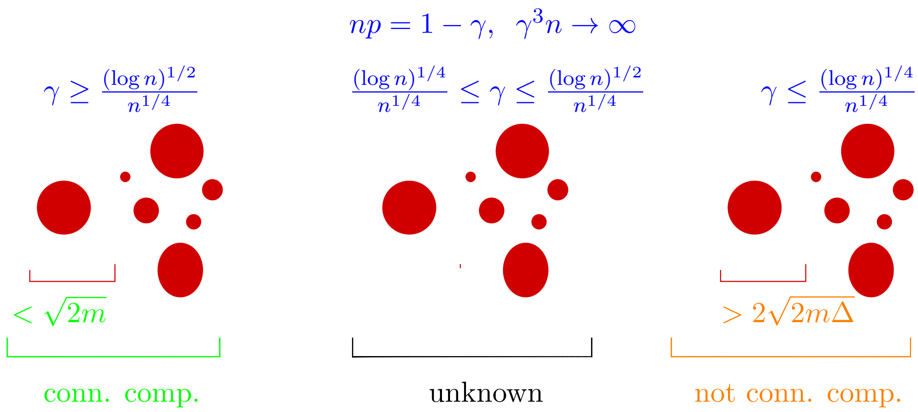


Figure 6.3: An illustration to accompany Theorem 6.1.5 showing which partition is whp optimal in the lower window of $\mathcal{G}(n,p)$ i.e. for $np = 1-\gamma$, $\gamma = o(1)$ and $\gamma^3 n \to \infty$. Also shown is the likely maximum numbers of edges within a connected component which imply these transitions, where m is the number of edges in the graph and Δ its maximum degree. Image credit for the circle illustration: Mihyun Kang, TU Graz, used with permission.

6.1.5 Concentration, Expectation and Stability

We also prove the modularity of a random graph is highly concentrated about its expectation in Theorem 6.6.1. An important open question is whether the expected modularity of $q^*(G_{n,c/n})$ tends to a limit $f(c)$ as $n \to \infty$. In Theorem 6.6.3 we show in this case the function $f(c)$ would be continous in c for $0 < c < \infty$.

6.1.6 Predictions from the literature

Predictions for the maximum modularity of Erdős-Rényi random graph have been made previously in the literature. Two papers, one by Reichardt and Bornholdt [56] and one by Guiméra et al. [27] have both conducted numerical simulations and used heuristics to predict the maximum modularity of Erdős-Rényi random graphs.

In [56], they make the assumption that any optimal partition will have parts of equal size. They then approximate the number of edges between parts using results from [33] where the authors give spin glass predictions for the number of crossing edges in an equipartition into k parts of an Erdős-Rényi random graph. Another heuristic from spin glasses is then used to determine a likely value for k. This and some simulations led them to predict that

$$q^*(G_n) \doteq 0.97\sqrt{\frac{1-p}{np}}. \tag{6.1}$$

A different approach is taken in [27]. They also assume that any optimal partition will be an equipartition, then make heuristic arguments that the maximum modularity will then be a function of np. Simulations were then undertaken to predict a rate of growth in terms of np and led them to predict[1],

$$q^*(G_n) \doteq \left(1 - \frac{1}{\sqrt{n}}\right)\left(\frac{1}{np}\right)^{2/3}. \tag{6.2}$$

In Theorem 6.1.1 we found three different phases of the likely maximum modularity. We proved for $np = 1 + o(1)$ the maximum modularity is $1 + o(1)$ whp and for $np \to \infty$ the maximum modularity is $o(1)$ whp. This confirms predictions (6.1) and (6.2) in this range to within 0.03 for large n. Note however, that the rate of convergence we prove is different to both predictions.

The likely maximum modularity of the random graph for $np \to c$ for some constant $c > 1$ is still somewhat open. We prove that that it lies between two positive functions $a(c) < b(c)$ where $b(c) \to 0$ as $c \to \infty$. In the language of [27], we roughly proved that the 'growth rate' in terms of np is somewhere between $-1/3$ and -1, i.e. $a(c) = c^{-1+o(1)}$ and $b(c) = c^{-1/3+o(1)}$, which compares to predicted 'growth rates' of $-2/3$ in [27] and $-1/2$ in [56].

[1] The prediction in the paper is actually $\left(1 - \frac{2}{\sqrt{n}}\right)\left(\frac{2}{np}\right)^{2/3}$ but this is based on a percolation point of $2/n$. If we instead suppose a percolation point of $1/n$ and adjust accordingly then the prediction is as in (6.2).

We mention one other related work from the literature. In Section 6.1.5 we study the expected maximum modularity of Erdős-Rényi random graphs. At first glance the results of that section may seem similar to work done by Franke [25]. However, where we look at the maximum modularity of a random graph, Franke's work considers the modularity of a random graph with respect to a uniformly chosen random vertex partition. The difference can be made clear by explicitly writing the expressions in each case. We study the expected maximum modularity of a random graph,

$$\mathbb{E}(q^*(G_n)) = \sum_{G \in \mathcal{G}_n} \mathbb{P}(G)(\max_{\mathcal{A}} q_{\mathcal{A}}(G)), \tag{6.3}$$

and Franke's work studies,

$$\sum_{G \in \mathcal{G}_n} \mathbb{P}(G) \sum_{\mathcal{A}} \mathbb{P}(\mathcal{A}) q_{\mathcal{A}}(G). \tag{6.4}$$

So while we both talk about the expected modularity of a random graph, we study the expected maximum modularity of a random graph (6.3) while Franke considers the expected modularity of a random partition of a random graph as in (6.4).

6.1.7 Outline

We begin by getting our hands dirty and prove results on the likely maximum modularity of particular vertex partitions. In Section 6.2 we determine the maximum modularity whp achieved by taking the parts to be the vertex sets of the connected components of our random graph in Lemma 6.2.1. We also give lower bounds for two alternate constructions for vertex partitions.

By the end of Section 6.2 we are ready to prove a result on the structure of the optimal partition, Theorem 6.1.5, which we do in Section 6.3 on p122.

After establishing lower bounds and properties of modularity in Sections 6.2 and 6.3 we are ready to prove our main result, the three phases of modularity, Theorem 6.1.1, in Section 6.4.

At the end of the chapter, we include an overview of known results of Erdős-Rényi random graphs in Section 6.7 beginning p145. The selection is biased by the properties we need to study modularity. It collects together the likely values for component sizes and number of edges and size of the giant component for different stages of the critical window and also in the supercritical range of the random graph.

6.2 Partitionology

In this section we describe three different construction techniques to create partitions of the vertex set of $\mathcal{G}(n,p)$ in the regime $np \to c$ and calculate lower bounds on the likely modularity of each. In Figure 6.4 we illustrate how these compare for small values of c.

In the case of the connected components partition an upper bound is also given and we will examine the maximum modularity for all possible p. We also show how the prune to forest construction performs in the regime of the young giant, for $p = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$.

Results in this section are important to complete the proof of Theorem 6.1.5 on p123.

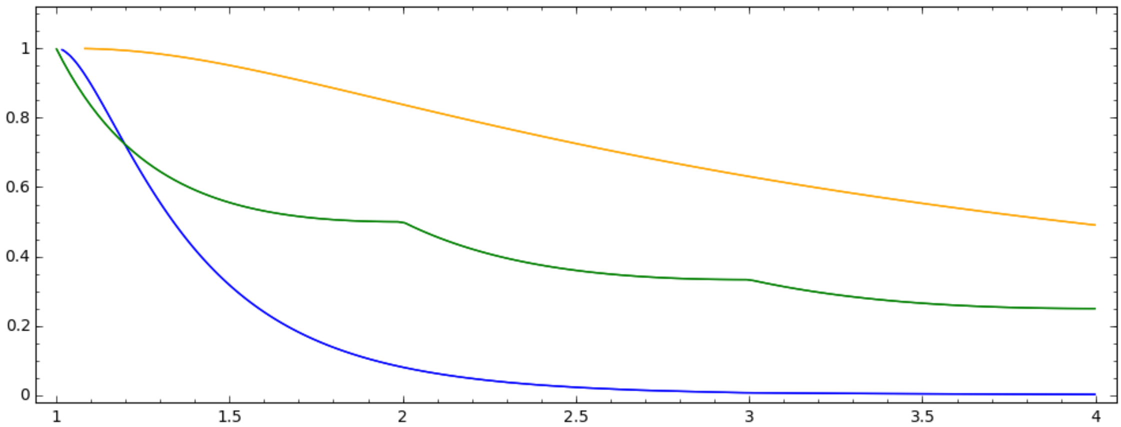


Figure 6.4: The graph shows the modularities of $\mathcal{G}(n, c/n)$ which are achieved whp by the prune-to-forest construction (in orange), the bootstrap construction (in green) and the connected components partition (in blue) for small values of $c > 1$ shown on the x-axis.

6.2.1 Connected components partition

For a graph G we let $\mathcal{CC} = \mathcal{CC}(G)$ be the partition whose parts are the vertex sets of the connected components of G. The next lemma provides detailed results on the likely modularity of the connected components partition of an Erdős-Rényi random graph. The focus of this section is to provide a proof of this lemma, part by part. The tables in Figures 6.5 and 6.6 summarise the parts of the lemma and display the page number of the proof.

If $n^2p \to \infty$ then whp $m \sim n^2p/2$. We choose to express our results in terms of n for the critical window and in terms of m before the critical window. However, the tables in Figures 6.5 and 6.6 show the results in terms of both parameters. Recall also, that for any graph G with $m > 0$ edges the degree tax of the connected components partition is at least $1/m$, by Corollary 1.4.2, so we do not state this lower bound explicitly in the lemma. Notice by definition the edge contribution of the connected components partition is always one, so $q_{\mathcal{CC}}(G) = 1 - q^D_{\mathcal{CC}}(G)$ and we can focus on the degree tax $q^D_{\mathcal{CC}}$.

We write $X_n \sim f(n)$ if $X_n = (1+o(1))f(n)$ and $X_n \preceq f(n)$ if $X_n \leq (1+o(1))f(n)$.

Lemma 6.2.1. *Let $p = p(n)$, suppose G_n is a random graph from $\mathcal{G}(n,p)$. Let $\mathcal{CC} = \mathcal{CC}(G_n)$ be the partition whose parts are the vertex sets of the connected components of G_n and m be the random variable $m = e(G_n)$.*

(i) If $n^2p \to \infty$ and $n^{3/2}p \to 0$, then whp $q^D_{\mathcal{CC}}(G_n) = \frac{1}{m}$.
(ii) If $n^2p \to \infty$ and $np = o(1)$ then whp $q^D_{\mathcal{CC}}(G_n) \preceq \frac{1}{m}$.
(iii) If $n^2p \to \infty$ and $np \preceq c$ for some constant $c < 1$, then whp

$$\frac{1}{m}\left(\frac{2}{1-np} - 1\right) \preceq q^D_{\mathcal{CC}}(G_n) \preceq \frac{1}{m}\left(\frac{2}{1-np} + 1\right).$$

(iv) If $np = 1-\gamma$ where $|\gamma| = o(1)$ and $\gamma^3 n \to \infty$, then whp $q^D_{\mathcal{CC}}(G_n) \sim \frac{4}{\gamma n}$.
(v) If $np = 1+\gamma$ where $\gamma = o(1)$ and $\gamma^3 n = O(1)$ then whp $q^D_{\mathcal{CC}}(G_n) = \Theta(\frac{1}{n^{2/3}})$.
(vi) If $np = 1+\gamma$ where $|\gamma| = o(1)$ and $\gamma^3 n \to \infty$, then whp $q^D_{\mathcal{CC}}(G_n) \sim 16\gamma^2$.
(vii) If $np \sim c$ for some constant $c > 1$, then whp $q^D_{\mathcal{CC}}(G_n) \sim (2\beta - \beta^2)^2$ where $\beta \in (0,1)$ satisfies $\beta + e^{-\beta c} = 1$.
(viii) If $np \to \infty$, then whp $q^D_{\mathcal{CC}}(G_n) = 1 - o(1)$.

We will prove each part of the lemma in order, pausing to compile the results which we need along the way. The following result of Erdős and Rényi from the very beginning of

range p	$q^D_{CC}(G_n)$ whp ...			
$n^{-2} \ll p \ll n^{-1}$	$\sim \frac{1}{m}$	$\sim \frac{2}{n^2p}$		p108
$n^{-2} \ll p \le \frac{c}{n}(1+o(1))\ \ c<1$	$\Theta(\frac{1}{m})$	$\Theta(\frac{1}{n^2p})$		p110
$p = \frac{1}{n}(1-\gamma), \gamma = o(1), \gamma^3 n \to \infty$	$\sim \frac{2}{\gamma m}$	$\sim \frac{4}{\gamma n}$	~ 0	p111
$p = \frac{1}{n}(1+\gamma), \gamma = o(1), \gamma^3 n = O(1)$	$\Theta(\frac{1}{m^{2/3}})$	$\Theta(\frac{1}{n^{2/3}})$		p112
$p = \frac{1}{n}(1+\gamma), \gamma = o(1), \gamma^3 n \to \infty$	$\sim 16\gamma^2$	$\sim 16\gamma^2$		p112
$p \sim \frac{c}{n},\ \ c>1$	$\sim (2\beta-\beta^2)^2$	$\sim (2\beta-\beta^2)^2$	$\sim (2\beta-\beta^2)^2$	p113
$p \gg n$	~ 1	~ 1	~ 1	p113

Figure 6.5: Table of asymptotic bounds which hold whp for the degree tax of the connected components partition, $q^D_{CC}(G_n)$.

range p	$q^D_{CC}(G_n)$ whp ...			
$n^{-2} \ll p \ll n^{-3/2}$	$* = \frac{1}{m}$			
$n^{-2} \ll p \ll n^{-1}$	$\frac{1}{m} \le * \preceq \frac{1}{m}$	$\sim \frac{1}{m}$	$\sim \frac{2}{n^2p}$	
$n^{-1} \ll p \ll cn^{-1}\ \ c<1$	$\frac{1}{m}(\frac{2}{1-np}-1) \preceq * \preceq \frac{1}{m}(\frac{2}{1-np}+1)$			
$p \sim cn^{-1}\ \ c<1$	$\frac{1}{m}(\frac{2}{1-c}-1) \preceq * \preceq \frac{1}{m}(\frac{2}{1-c}+1)$	$\Theta(\frac{1}{m})$	$\Theta(\frac{1}{n^2p})$	~ 0

Figure 6.6: Table of asymptotic bounds which hold whp for the degree tax of the connected components partition, $q^D_{CC}(G_n)$, precise results for small p. We write $*$ to abbreviate $q^D_{CC}(G_n)$.

random graphs [22], will be useful to prove part (i) and part of the range for p in part (ii) of Lemma 6.2.1.

Lemma 6.2.2 (Erdős-Rényi [22])**.** *Fix a graph H and write $\rho(H) = \max_{H' \subseteq H} e(H')/|H'|$. If $n^{\rho(H)}p \to 0$ then whp G_n does not contain H as a subgraph.*

The proof of this lemma follows by the first moment method, one calculates the expected number of H' in G_n and show that this tends to 0 for any H' subgraph of H. This lemma along with Corollary 1.4.2 will allow us to prove part (i).

Proof. (of Lemma 6.2.1(i)) **(Case:** $n^2p \to \infty$ and $n^{3/2}p \to 0$.**)**
We first need to esablish that whp the graph G_n will have edges. Write m for the random variable $m = e(G_n)$. By Chernoff, Lemma 6.4.4 using $\delta = 1/2$, $\mathbb{P}(m \leq \mathbb{E}[m]/2) \leq \exp(-\mathbb{E}[m]/8)$. Now note that $n^2p \to \infty$ implies $\mathbb{E}[m] \to \infty$, and hence whp $m > \mathbb{E}[m]/2$. In particular, whp $m \geq 1$ and the modularity of G_n is defined.

By Lemma 6.2.2, $n^{2/3}p \to 0$ implies whp G_n will not contain the path on three vertices as a subgraph and so whp G_n consists of disjoint edges. Hence by Lemma 1.4.2 whp $q^D_{CC}(G_n) = 1 - \frac{1}{m}$ and we are done. □

For the proofs of parts (ii) and (iii) we introduce the graph parameter $\chi(G)$, sometimes referred to as susceptibility in the literature. The parameter $\chi(G)$ tracks the sum of the squares of component sizes in G. The usual quantity that is meant by susceptibility for a *random graph* G_n is $\mathbb{E}(\chi(G_n))$ which is often used in percolation theory. However, Janson and Luczak study $\chi(G_n)$ (and not $\mathbb{E}(\chi(G_n))$) for an Erdős-Rényi random graph G_n in [30] and refer to it as susceptibility, see Lemma 6.2.6.

Definition 6.2.1 (susceptibility $\chi(G)$)**.** *For a graph G with n vertices denote by $C_1, \ldots, C_k$ the vertex sets of the connected components of G. Then define*

$$\chi(G) = \frac{1}{n} \sum_{i=1}^{k} |C_i|^2.$$

For $v \in V(G)$ denote by c_v the size of the connected component containing v. For a graph G, let $X = X(G)$ denotes the size of the component containing a vertex picked uniformly at random. Then $\mathbb{E}(X) = \frac{1}{n} \sum_{u \in V} c_u = \frac{1}{n} \sum_i |C_i|^2 = \chi(G)$. Hence, for any fixed graph G, the susceptibility $\chi(G)$ describes the expected size of the connected component of a vertex picked uniformly at random from $V(G)$.

The degree tax of the connected components partition can be expressed in terms of this parameter $\chi(G)$ and the excesses of the connected components of G. Recall the excess of a connected component C is $\ell(C) = e(C) - |C|$. Note if C is a tree then $\ell(C) = -1$. The excess of a graph is the sum of the excesses of its non-tree connected components, i.e. $\ell(G) = \sum_{C:\ell(C)\geq 0} \ell(C)$.

Lemma 6.2.3. *Let G be a graph and let $C_1, \dots, C_k$ be the vertex sets of the connected components of G. Further, let t_c be the number of tree components of G and let t_v be the number of vertices in tree components of G. Then*

$$q^D_{CC}(G) = \frac{1}{m^2}\left(n\chi(G) - 2t_v + t_c + \sum_{i:\ell(C_i)>0} \ell(C_i)(|C_i| + e(C_i))\right).$$

Proof. This is a matter of checking.

$$\begin{aligned}
q^D_{CC}(G) &= \frac{1}{m^2}\sum_i e(C_i)^2 \\
&= \frac{1}{m^2}\Big(\sum_{i:\ell(C_i)=-1}(|C_i|-1)^2 + \sum_{i:\ell(C_i)=0}|C_i|^2 + \sum_{i:\ell(C_i)>0}(|C_i| + \ell(C_i))^2\Big) \\
&= \frac{1}{m^2}\Big(\sum_i |C_i|^2 + \sum_{i:\ell(C_i)=-1}(-2|C_i|+1) + \sum_{i:\ell(C_i)>0}\ell(C_i)(2|C_i| + \ell(C_i))\Big) \\
&= \frac{1}{m^2}\Big(n\chi(G) - 2t_v + t_c + \sum_{i:\ell(C_i)>0}\ell(C_i)(|C_i| + e(C_i))\Big).
\end{aligned}$$

□

We note two implications of this lemma. Recall for a forest on n vertices with m edges the number of components is $n - m$, and the first corollary is immediate.

Corollary 6.2.4. *If G is a forest then*

$$q^D_{CC}(G) = \frac{1}{m^2}\left(n\chi(G) - n - m\right).$$

The second corollary is useful in the proofs of part (iii).

Corollary 6.2.5. *Let G be a graph with m edges, n vertices and excess $\ell(G) = \ell$ then*

$$\frac{1}{m^2}\left(n\chi(G) - n - m + \ell\right) \le q_{\mathcal{CC}}^D(G) \le \frac{1}{m^2}\left(n\chi(G) - n + m - \ell\right) + \frac{2\ell}{m}.$$

Proof. We can give a detailed expression for the number of edges in G,

$$m = \sum_{A\in\mathcal{CC}} e(A) = \sum_{\ell(A)=-1}\big(|A|-1\big) + \sum_{\ell(A)=0}|A| + \sum_{\ell(A)>0}\big(|A|+\ell(A)\big) = n - t_c + \ell.$$

Hence the number of tree components is $t_c = n - m + \ell$. Also note that $t_v \ge t_c$ and that $t_v \le n$. These three observations together imply that $-n-m+\ell \le -2t_v + t_c \le -n+m-\ell$. We now examine the last term in Lemma 6.2.3, noting that components C with $\ell(C) > 0$ will satisfy $|C| \le e(C)$,

$$\sum_{i:\ell(C_i)>0} \ell(C_i)(|C_i| + e(C_i)) \le 2\sum_{i:\ell(C_i)>0} \ell(C_i)e(C_i) \le 2\ell m.$$

and we are done. □

The value of $\chi(G)$ is well understood for subcritical random graphs. We will use the following result by Janson and Luczak which appears as Theorem 1.1 in [30].

Lemma 6.2.6 (Janson and Luczak [30])**.** *Let $0 \le p < 1/n$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Then whp*

$$\chi(G_n) = \frac{1}{1-np}\left(1 + O\left(\frac{1}{\sqrt{n(1-np)^3}}\right)\right).$$

The next proof also uses Markov's inequality so we recall it below.

Lemma 6.2.7 (Markov's inequality)**.** *Let Y be a non-negative random variable and fix $\alpha > 0$. Then $\mathbb{P}[Y > \alpha\mathbb{E}(Y)] < \frac{1}{\alpha}$.*

We are now ready to continue to the proof of the next part of Lemma 6.2.1.

Proof. (of Lemma 6.2.1(ii)) **(Case:** $n^2p \to \infty$ and $np = o(1)$.**)**
Fix $\varepsilon > 0$. Observe that $\mathbb{E}[m] = \binom{n}{2}p \to \infty$ and so by Chernoff, Lemma 6.4.4, whp $|m - \mathbb{E}[m]| < \varepsilon\mathbb{E}[m]/3$. This implies that whp $|\frac{1}{m} - \frac{2}{n^2p}| < \frac{2\varepsilon}{n^2p}$ and so it will be sufficient to show that whp $\frac{1}{m} \le q_{\mathcal{CC}}^D(G) = \frac{1}{m}(1+o(1))$. The lower bound follows by Lemma 1.4.2.

For the upper bound we split into two ranges of p. Range 1 covers $n^2p \to \infty$ and $n^{4/3}p = o(1)$ and uses subgraph counts and Range 2 covers $n^{3/2}p \to \infty$ and $np = o(1)$ and uses results on susceptibility.

Range 1: $n^2p \to \infty$ and $n^{4/3}p = o(1)$.
By Lemma 6.2.2, as $np = o(1)$ whp G_n does not contain a triangle as a subgraph and as $n^{4/3}p = o(1)$ whp G_n does not contain the path on four vertices as a subgraph. Hence whp G_n consists of connected components which are isolated vertices, single edges or the path on three vertices. The isolated vertices have no degree so are not included in the degree tax and we can ignore them. Write Y to be the number of paths on three vertices and we can express the degree tax in terms of m and Y

$$q^D_{CC} = \frac{1}{4m^2}(2^2(m-2Y)+4^2Y) = \frac{1}{m}(1+2Y/m) \tag{6.5}$$

Notice the expected number of paths on three vertices is $\mathbb{E}(Y) = \binom{n}{3}3p^2 \leq n^3p^2$. Now we can use Markov's inequality: Lemma 6.2.7.

$$\mathbb{P}(Y > \alpha n^3p^2) \leq \mathbb{P}(Y > \alpha\mathbb{E}[Y]) < \frac{1}{\alpha}.$$

If we take $\alpha = (n^2p)^{1/10}$ then $\alpha \to \infty$ and so by Markov whp $Y \leq (n^2p)^{1/10}n^3p^2$. This implies whp $2Y/m = O((n^2p)^{-9/10}n^3p^2) = O((n^{12/11}p)^{11/10}) = o(1)$ and so by (6.5) we are done. This proves case 1.

Range 2: $n^{3/2}p \to \infty$ and $np = o(1)$.
Note that whp G_n has no cycles and so by Lemma 6.2.4, whp the following holds

$$q^D_{CC}(G) = \frac{1}{m^2}(n\chi(G) - n - m).$$

Now substitute the result of Janson and Luczak in Lemma 6.2.6 and do a little rearranging to obtain:

$$\begin{aligned} m^2q^D_{CC}(G) &= \frac{n}{1-np}\left(1+O(n^{-1/2})\right) - n - m \\ &= \frac{1}{1-np}\left(n^2p - m + mnp + O(n^{1/2})\right). \end{aligned}$$

As earlier observed $n^2p = 2m(1+o(1))$,

$$m^2q^D_{CC}(G) = \frac{1}{1-np}\left(m(1+o(1)) + mnp + O(n^{1/2})\right).$$

Also, $np = o(1)$ implies $mnp = o(m)$ and that the denominator is $1 + o(1)$. Hence,

$$m^2 q^D_{CC}(G) \quad = \quad \Big(m + O(n^{1/2})\Big)\,(1 + o(1)). \tag{6.6}$$

Lastly examine the $O(n^{1/2})$ term. We know $m = n^2p(1+o(1))/2$, so $n^{1/2}/m = 2n^{-3/2}p^{-1}(1+o(1))$. But $n^{3/2}p \to \infty$ which means $n^{1/2} = o(m)$. Hence by (6.6) we are done. □

Proof. (of Lemma 6.2.1(iii)) **(Case:** $n^2p \to \infty$ and $np \le c + o(1)$ for some constant $c < 1$.**)**

In this range, whp all connected components in G_n are trees or unicyclic by Lemma 6.7.1, so whp $\ell(G_n) = 0$. Hence by Corollary 6.2.5 whp

$$\frac{1}{m^2}(n\chi(G_n) - n - m) \le q^D_{CC}(G_n) \le \frac{1}{m^2}(n\chi(G_n) - n + m). \tag{6.7}$$

Simplifying the common part of the upper and lower bound, $\frac{1}{m^2}(n\chi(G_n) - n)$, we begin by noting whp $2m = n^2p(1+o(1))$ and substituting the expression for $\chi(G_n)$ from Lemma 6.2.6.

$$\begin{aligned}
\frac{1}{m^2}(n\chi(G_n) - n) &= \frac{2}{mnp}(\chi(G_n) - 1)(1 + o(1)) \\
&= \frac{2}{mnp}\bigg(- 1 + \frac{1}{1 - np} + O(n^{-1/2})\bigg)(1 + o(1)) \\
&= \frac{2}{m(1 - np)}(1 + o(1))
\end{aligned}$$

Thus by (6.7), we can write the upper and lower bounds for the degree tax of the connected components partition of G_n.

$$\frac{1}{m}\bigg(\frac{2}{1 - np} - 1\bigg)(1 + o(1)) \le q^D_{CC}(G_n) \le \frac{1}{m}\bigg(\frac{2}{1 - np} + 1\bigg)(1 + o(1)).$$

□

We will often need to bound the likely number of edges in a random graph.

Lemma 6.2.8. *Let* $0 < c_0 < \infty$, $\omega = \omega(n) \to \infty$ *and* $p = p(n)$ *satisfy* $c_0 < np$ *and* $G_n \sim (n, p)$. *Write* $m = e(G_n)$, *then whp*

$$\Big|m - \binom{n}{2}p\Big| < \frac{\omega\binom{n}{2}p}{\sqrt{n}}.$$

Proof. By Chernoff, Lemma 6.4.4,

$$\begin{aligned}\mathbb{P}\left(\left|m-\binom{n}{2}p\right|>\delta\binom{n}{2}p\right) &\leq 2\exp\left(-\frac{\delta^2\mathbb{E}(m)}{2(1+\delta/3)}\right)\\ &= 2\exp\left(-\frac{\delta^2 n(n-1)p}{4(1+\delta/3)}\right)\end{aligned}$$

Thus it is sufficient if $\frac{\delta^2(n-1)}{4(1+\delta/3)} \to \infty$ as $n \to \infty$. Take $\delta = \omega/\sqrt{n}$ and we are done. □

Proof. (of Lemma 6.2.1(iv))**(Case:** $np = 1-\gamma$ where $|\gamma| = o(1)$ and $\gamma^3 n \to \infty$.**)**
For this range of p whp $\ell(G) = 0$ by Lemma 6.7.1. Hence by Corollary 6.2.5

$$\frac{1}{m^2}\left(n\chi(G)-n-m\right) \leq q^D_{CC}(G) \leq \frac{1}{m^2}\left(n\chi(G)-n+m\right)$$

The susceptibility $\chi(G)$ by Lemma 6.2.6 is $\chi(G) = \frac{1}{\gamma}(1+O(\frac{1}{(\gamma^3 n)^{1/2}})) = \frac{1}{\gamma}(1+o(1))$, where the second inequality is because $\gamma^3 n \to \infty$. Now by Lemma 6.2.8 whp $m = n^2 p(1+o(1))/2 = n(1+o(1))/2$. Hence whp

$$\frac{n\chi(G)}{m^2} = \frac{4}{n\gamma}(1+o(1)).$$

It is now sufficient to show that $(n+m)/m^2 = o(1/(n\gamma))$, i.e. that $n\gamma(n+m)/m^2 = o(1)$. But this easily follows because $m = \Theta(n)$ and $\gamma = o(1)$ and so we are done. □

In the appendix of [30], Janson and Luczak prove two results: Theorems A1 and B1, on the susceptibility in the upper window and in the critical case.

Lemma 6.2.9 (Janson and Luczak [30])**.** *Let $np = 1+\gamma$ where $\gamma = o(1)$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Then whp, denoting by $C_1 = C_1(G_n)$ the largest connected component of G_n,*

$$\chi(G_n) = \begin{cases}\Theta(n^{1/3}) & \text{if } \gamma^3 n = O(1)\\ \dfrac{|C_1|^2}{n} + O\left(\dfrac{1}{\gamma}\right) & \text{if } \gamma^3 n \to \infty.\end{cases}$$

The proof of Lemma 6.2.1 in the critical case, part (v), is almost immediate from Lemma 6.2.9.

Proof. (of Lemma 6.2.1(v)) **(Case:** $np = 1+\gamma$, $\gamma = o(1)$ and $\gamma^3 n = O(1)$.**)**
First recall by Lemma 6.7.2 whp $\ell(G_n) = O(1)$. This lets us relate the sum of squares of the edges in our components to the susceptibility

$$\sum_i e(C_i)^2 = \sum_i (|C_i| + \ell(C_i))^2 = \sum_i |C_i|^2 + O(n) = n\chi(G_n) + O(n). \tag{6.8}$$

Whp by Lemma 6.2.9, $\chi = \Theta(n^{1/3})$ and by Lemma 6.2.8 $m = \Theta(n)$ and so

$$q^D_{CC} = \frac{1}{m^2}\sum_i e(C_i)^2 = \Theta\left(\frac{1}{n^{2/3}}\right),$$

and we are done. □

Proof. (of Lemma 6.2.1(vi)) **(Case:** $np = 1+\gamma$, $\gamma = o(1)$ and $\gamma^3 n \to \infty$.**)**
Denote the connected components of G_n by $C_1, \ldots, C_k$ where $|C_1| \geq |C_2| \geq \ldots \geq |C_k|$. We first **claim** that whp

$$\sum_i e(C_i)^2 = e(C_1)^2 + O\left(\frac{n}{\gamma}\right). \tag{6.9}$$

To show this claim, first notice that whp by Lemma 6.7.3, for $\forall i > 1$, $\ell(C_i) \in \{-1, 0\}$. And so $\sum_{i>1} e(C_i)^2 \leq \sum_{i>1} |C_i|^2$. Hence $\sum_i e(C_i)^2 \leq e(C_1)^2 - |C_1|^2 + n\chi(G)$ and the claim (6.9) follows by Lemma 6.2.9.

We now make an estimate of $e(C_1)^2/m^2$. Let $\omega(n) \to \infty$. By Lemmas 6.2.8 and 6.7.7, whp $m = n(1+\gamma+O(\omega n^{-1/2}))/2$ and

$$e(C_1) = 2\gamma n\left(1 - \frac{4\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right).$$

Thus, with some rearranging, whp

$$\begin{aligned}
\frac{e(C_1)^2}{m^2} &= \frac{16\gamma^2}{(1+\gamma+O(\frac{\omega}{\sqrt{n}}))^2}\left(1 - \frac{4\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right)^2 \\
&= 16\gamma^2\left(1 - \frac{8\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right)\left(1 - 2\gamma + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{n}}\right)\right) \\
&= 16\gamma^2\left(1 - \frac{14\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right).
\end{aligned} \tag{6.10}$$

For the error term in (6.9), note $\gamma^3 n \to \infty$ implies $\frac{1}{\gamma n} = o(\gamma^2)$ and so whp $\frac{n}{\gamma m^2} = o(\gamma^2)$. Hence by (6.9) and (6.10) whp

$$q_{CC}^D(G_n) = \frac{\sum_i e(C_i)^2}{m^2} = 16\gamma^2\left(1 - \frac{14\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right) + o(\gamma^2) = 16\gamma^2(1 + o(1)),$$

and the proof is complete. $\square$

It will be useful later, in Theorem 6.1.5, to prove a slightly more general lemma which then implies part (vii) of Lemma 6.2.1.

Lemma 6.2.10. *Suppose $\exists n_0$ such that $\forall n > n_0$, $k \leq np \leq K$ for some constants $k, K > 1$ and suppose $G_n \sim \mathcal{G}(n,p)$. Write $c = np$ and define $t \in (0,1)$ by $te^{-t} = ce^{-c}$. Then whp*

$$q_{CC}^D(G_n) = 1 - \frac{2t^2}{c^2} + \frac{t^4}{c^4} + o(1).$$

Proof. Whp G_n has a giant component H. We first calculate the degree tax associated with H. We know the edge count inside H to be $e(H) = (1 - t/c)(c+t)n(1+o(1))/2$ by Lemma 6.7.5 and the number of edges in G_n to be $m = cn(1+o(1))/2$. Thus,

$$\frac{e(H)^2}{m^2} = \frac{(1-t/c)^2(c+t)^2 n^2}{c^2 n^2}(1+o(1)) = 1 - \frac{2t^2}{c^2} + \frac{t^4}{c^4} + o(1).$$

It now suffices to show that the contribution of all other parts to the degree tax is $o(1)$. Recall that by Lemma 6.1.2 whp the number of edges in each other connected component is $O(\log n)$. Observe if $0 < x_i = O(\log n)$ and $\sum_i x_i \leq 2m$ then $\sum_i x_i^2 = O(m \log n)$. Therefore we can bound the contribution these parts make to the degree tax, whp

$$q_{CC}^D(G_n) - \frac{e(H)^2}{m^2} = O(\frac{\log n}{m}) = O(\frac{\log n}{n}) = o(1)$$

and we are done. $\square$

Proof. (of Lemma 6.2.1(vii)) **(Case:** $np = c + o(1)$ for some constant $c > 1$.**)**
This result is implied by Lemma 6.2.10. $\square$

Proof. (of Lemma 6.2.1(viii)) **(Case:** $np \to \infty$.**)**
This result follows from some facts on the size of the giant component in this range. Fix $0 < \varepsilon < 1/3$ and it will suffice to show that whp $q_{CC}^D(G_n) \geq 1 - \varepsilon$. We can choose $c' = c'(\varepsilon)$ large enough so that $\beta > 1 - \varepsilon/3$, where $\beta \in (0,1)$ is a solution of $\beta + e^{-\beta c'} = 1$. Hence for $p = c'/n$ whp the giant component has at least $(1-\varepsilon/3)(1+o(1))n$ vertices by Lemma 6.7.4.

Note as edges are added to a graph the number of vertices in the giant component cannot decrease and so whp the giant component of G_n, call it H, satisfies $|H| \geq (1-\varepsilon/3)(1+o(1))n$.

By Lemma 6.7.1 all other components are trees or unicyclic and so have average degree at most 2. Thus the number of edges not in the giant component is at most $\varepsilon n/3$.

We can now bound $e(H)$ by $e(H) \geq m - \varepsilon n/3$, and so (noticing $2m = n^2 p(1+o(1))$ implies $n < m$),

$$q^D_{CC}(G_n) \geq \frac{e(H)^2}{m^2} \geq \left(1 - \frac{\varepsilon n}{3m}\right)^2 \geq (1-\varepsilon/3)^2 \geq 1-\varepsilon,$$

and we are done. □

The functions (in terms of c) of the likely component size $\sim (1-t/c)n$ and modularity of connected components partition $\sim 1 - \frac{2t^2}{c^2} + \frac{t^4}{c^4}$ are illustrated in Figure 6.2.1. For $c = 2$ this gives maximum modularity just a little above 0.08, for $c = 3/2$ it gives maximum modularity approx 0.32 and for $c = 5/4$ it gives modularity a little above 0.63.

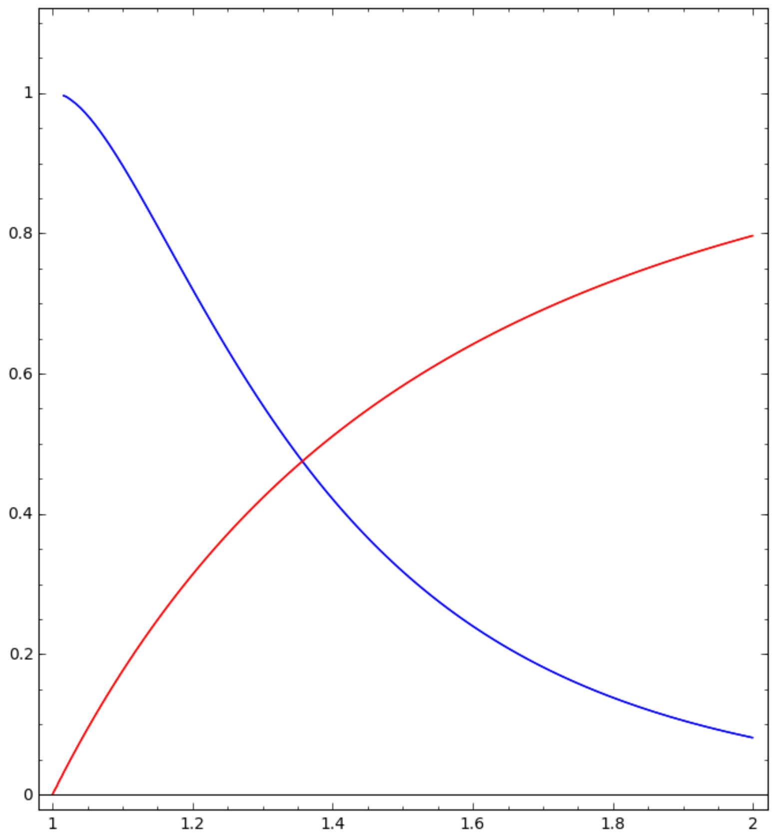


Figure 6.7: The graph shows the size of giant component as a ratio of the number of edges (in red) and the modularity achieved whp by the connected components partition (in blue) in the random graph $\mathcal{G}(n, c/n)$ for values of c shown on the x-axis. This follows from the result in Lemma 6.2.1(v).

6.2.2 Bootstrap/Multiple Exposure Construction

This *bootstrap* or *multiple exposure* construction lets us 'bootstrap' from high modularity partitions for $p = 1/n$ into higher values of p. It relies on the following observation.

Sampling a random graph on n vertices with edge probability $p = 2/n$ is like taking two graphs on $n' = n/2$ vertices with edge probability $1/n'$ and then exposing the edges between the two halves with edge probability $2/n$.

Before we expose the edges between the two, each half is an Erdős-Rényi random graph at criticality and so whp it has components of size $\Theta(n'^{2/3})$ and many small parts of size $O(\log(n'))$. Hence in each half we can group these connected components into a large constant number of parts of nearly equal size. This will ensure edge contribution one and small degree tax. Keep that same vertex partition. When we expose the edges in between we doubled the total number of edges in the graph, but didn't get any more within our parts, so our edge contribution is 1/2. However, we can show that whp the added edges fell relatively evenly between the parts and so our degree tax is still negligible.

This idea extends to higher c by breaking the graph into more pieces, and exposing inside those first, picking a partition, then exposing between the pieces. For technical reasons we divide our original graph into parts of size n' slightly smaller so that the effective edge probability (considered as a graph on n' vertices) is slightly less than $1/n'$. However the idea is the same.

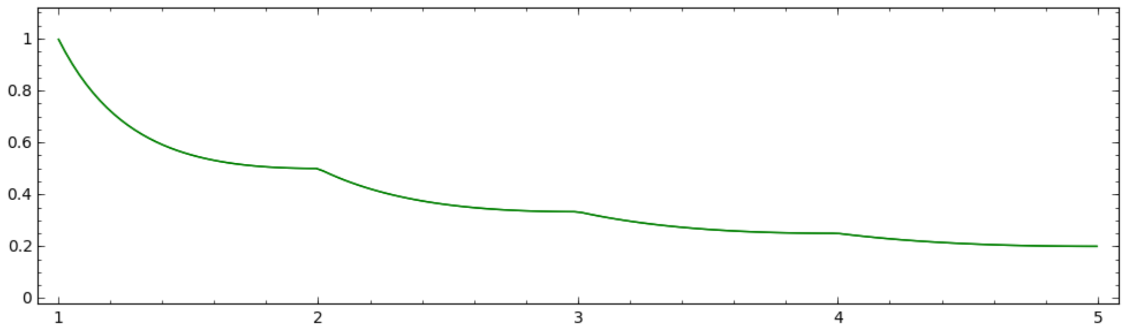


Figure 6.8: The graph shows the modularities of $\mathcal{G}(n, c/n)$ which are achieved whp by the bootstrap construction (in green) for small values of c as shown on the x-axis. The function plotted is provided by Theorem 6.2.11.

Theorem 6.2.11. *Fix $c > 1$ and write $c = k + \delta$ for k an integer and $\delta \in [0, 1)$. Suppose G_n is a random graph from $\mathcal{G}(n, c/n)$. Then whp $q^*(G_n) \geq \frac{k+\delta^2}{(k+\delta)^2} + o(1)$.*

Note that Theorem 6.2.11 implies that for $p = c/n$ whp $q^*(G_n) > \frac{1}{c+1}$. We will need the next lemma to help us track the degree tax increase after the second round of edge exposure in the proof of the theorem.

Lemma 6.2.12. *Fix positive integers h and k, a real $\delta \in [0, 1)$ and vertex sets U V, where $|U| \leq \frac{n}{(k+\delta)h}$ and $|V| \leq n$. Let G be the random graph generated by adding each possible edge between U and V independently with probability $p = (k + \delta)/n$. Then for large enough n,*

$$\mathbb{P}\Big(e(U, V) > \frac{n}{h}(1 + n^{-1}\log n)\Big) < \frac{1}{\log n}.$$

Proof. First observe that it is sufficient to prove this statement for $|U| = \frac{n}{(k+\delta)h}$ and $|V| = n$ and in this case that the expected number of edges is n/h. Hence by Chernoff -

$$\mathbb{P}\Big(e(U, V) > \frac{n}{h}(1 + \delta)\Big) \leq \exp\Big(\frac{-\delta^2 n}{2h(1 + \delta/3)}\Big)\Big). \tag{6.11}$$

Note that for $\delta < 1$, $\frac{\delta^2 n}{2h(1+\delta/3)} > \delta n/(4h)$ and so for large enough n it is sufficient to choose δ such that $\delta n/(4h) > \log\log n$. Hence we can take $\delta = n^{-1}\log n$ to complete the proof. □

We are now ready to prove Theorem 6.2.11.

Proof. (of Theorem 6.2.11) Fix an integer h such that $6/(h(k + \delta)) < \varepsilon$.

Let $a = \lfloor (n - n^{2/3}\log n)/(k+\delta) \rfloor$, and split the vertex set into $k+1$ sets $|V_1| = |V_2| = \ldots = |V_k| = a$ and V_{k+1} contains the remaining vertices from $[n]$.

We sample a graph with edge probability $(k + \delta)/n$ on the vertex set $V_1 \cup \ldots \cup V_{k+1}$ by exposing the edges in two rounds. In the first round we expose edges with both end points in one of the V_i's, in the second round we expose edges between the sets V_i and V_j for $i \neq j$.

Fix $i \leq k$ and begin by examining the graph induced on V_i i.e. $G|_{V_i}$ after the first exposure which is distributed as $\sim G(a, (1 - a^{-1/3}\log a)/a)$. Hence by Lemma 6.1.2 and Lemma 6.7.1 whp in $G|_{V_i}$ all connected components are of size $O(\log n)$ with excess either 0 or 1. So whp we can group these connected components into an h part vertex partition $\mathcal{A}_i$ of V_i such that all edges in $G|_{V_i}$ fall within parts, and $\forall A \in \mathcal{A}_i$,

$$|A| < \frac{n - n^{2/3}\log n}{(k+\delta)h} + (\log n)^2 \leq \frac{n}{(k+\delta)h} \text{ and } e(A) \leq |A|. \tag{6.12}$$

Similarly we have partitions $\mathcal{A}_j$ for $j = 1, \ldots, k$ with the same two properties. Consider the remaining vertices in V_{k+1}. The size of this vertex subset is $b = n - ka \leq \frac{n}{k+\delta}(\delta + n^{-1/3}\log n + 1)$. Hence after the first exposure the graph $G|_{V_{h+1}}$ is distributed as $\sim G(b, \delta + n^{-1/3}\log n + 1)$ and so whp all connected components are of size $O(\log n)$ with excess either 0 or 1. And, as above, we can create a partition $\mathcal{A}_{k+1}$ so that all edges in $G|_{V_{k+1}}$ fall within parts and $\forall A \in \mathcal{A}_{k+1}$ the properties in (6.12) hold.

We now expose the edges between vertex subsets $V_1, \ldots, V_{k+1}$. As each part has size and edges bounded as in (6.12) we can bound the likely degree sum of any part after the second exposure using Lemma 6.2.12. In particular, whp $\forall A \in \cup_{i=1}^k \mathcal{A}_i$

$$\mathrm{ds}(A) \leq 2|A| + \frac{n}{h}(1 + n^{-1}\log n) = \frac{n}{h}\left(1 + \frac{2}{k+\delta} + \frac{\log n}{\sqrt{n}}\right) \tag{6.13}$$

We let $\mathcal{A} = \cup_i \mathcal{A}_i$ be a partition of V and thus the degree tax of $\mathcal{A}$ must be at most the quantity in (6.13) divided by $2m$. Thus whp,

$$q_{\mathcal{A}}^D(G_n) \leq \frac{1}{h(k+\delta)}\left(1 + \frac{2}{k+\delta} + \frac{\log n}{\sqrt{n}}\right) \leq \frac{3}{h(k+\delta)} < \varepsilon/2.$$

Then, because all edges of the first exposure fall within parts by design of our $\mathcal{A}$ we get whp

$$q_{\mathcal{A}}^E(G_n) = \frac{k+\delta}{n}\left(k\binom{a}{2} + \binom{b}{2}\right)\frac{2}{(k+\delta)n}(1+o(1)) = \frac{k+\delta^2}{(k+\delta)^2}(1+o(1)) \geq \frac{k+\delta^2}{(k+\delta)^2} - \varepsilon/2$$

and we have proved our result. □

6.2.3 Prune-to-Forest Construction

We define a *prune-to-forest* construction which yields a higher modularity than the components partition in some regimes of p. Shortly after the giant component emerges it is possible to remove a small number of edges to leave it a tree. This tree also has low maximum degree and so we can partition the giant component nicely into parts, and, setting the other parts as the vertex sets of the non-giant connected components in the graph we create a partition of high modularity.

We begin with a reminder of a general lemma that relates the total number of edges (h) in the component (H) of the graph that needs pruning, the number of edges we need to prune ($\ell = |H| - h$), maximum degree (Δ) and total number of edges in the graph (m). With these parameters we can determine a lower bound on how well our *prune-to-forest* partition will perform. Technically we prune to a disjoint union of trees and unicyclic components. By Lemma 3.2.2 for $s > 2\Delta$,

$$q_{\mathcal{PF}}(H, m) \geq \frac{h}{m} - \frac{\ell}{m} - \frac{4h\Delta}{sm} - \frac{h(s-1)}{2m^2}$$

This gives a lower bound for how well we can partition connected components which are 'close' to a tree. We begin by bounding the likely maximum degree of a random graph, a simple result we will use many times in this chapter.

Lemma 6.2.13. *Suppose $0 < c_1 < \infty$ and $p(n)$ is such that $np < c_1$. Let $G_n \sim \mathcal{G}(n,p)$. Then whp $\Delta(G_n) < 2\log n / \log\log n$.*

Proof. Fix a vertex v. Then

$$\mathbb{P}(\deg(v) \geq k) \leq \binom{n}{k} p^k \leq \left(\frac{enp}{k}\right)^k = \exp\big(-k(\log k + O(1))\big)$$

and this is $o(1/n)$ if $k = 2\log n/\log\log n$ and so the result follows by the union bound. □

Theorem 6.2.14. *Let $np = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Then whp*

$$q^*(G_n) \geq 1 - \left(\frac{4\gamma^3}{3} - 16\gamma\sqrt{\frac{\log n}{n \log\log n}}\right)(1 + o(1)).$$

Proof. Write $m = e(G_n)$ and $d = \Delta(G_n)$. Then whp G_n has a unique giant component (say H). We denote the edges by $h = e(H)$. By our technical lemma in Chapter 3, Lemma 3.2.2, for $s > 2d$,

$$q_{\mathcal{PF}}(H,m) \geq \frac{h}{m} - \frac{\ell}{m} - \frac{2h(t+1)d}{sm} - \frac{h(s-1)}{2m^2} \tag{6.14}$$

Note we can set $s = 2\sqrt{2dm}$ (and whp it satisfies $s > 2d$). With this value of s substituted into (6.14) we deduce that whp,

$$q_{\mathcal{PF}}(H,m) \geq \frac{h}{m} - \frac{\ell}{m} - \frac{\sqrt{2}h(t+1)\sqrt{d}}{m^{3/2}}. \tag{6.15}$$

We now turn to analysing (6.15). Using the likely ranges for h and m in the previous paragraph we can bound the last term -

$$\frac{\sqrt{2}h(t+1)\sqrt{d}}{m^{3/2}} \leq \frac{\sqrt{2}\cdot 2\gamma n \cdot 2 \cdot \sqrt{d}}{(n/2)^{3/2}} = \frac{16\gamma\sqrt{d}}{\sqrt{n}}(1+o(1)).$$

Now, whp the excess $\ell(H) \leq 2\gamma^3 n(1+o(1))/3$ by Corollary 6.7.8 and thus by (6.15),

$$\frac{h}{m} - q_{\mathcal{PF}}(H,m) \leq \left(\frac{4\gamma^3}{3} + \frac{16\gamma\sqrt{d}}{\sqrt{n}}\right)(1+o(1)),$$

which can be simplified into the following expression by the likely bound on maximum degree in Lemma 6.2.13,

$$\frac{h}{m} - q_{\mathcal{PF}}(H,m) \leq 4\gamma\left(\frac{\gamma^2}{3} + 4\sqrt{\frac{\log n}{n\log\log n}}\right)(1+o(1)),$$

and because the contribution to the degree tax of the non-giant components will be negligible we have completed the proof. □

Theorem 6.2.15. *Let $np \to c$ where $c > 1$ is a constant and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Let $t \in (0,1)$ satisfy $te^{-t} = ce^{-c}$, then whp*

$$q_{\mathcal{PF}}(G_n) \geq \frac{2}{c} - \frac{t(2-t)}{c^2} + o(1).$$

To prove this theorem we will actually proceed by stating and proving a slightly more general lemma.

Lemma 6.2.16. *Suppose $\exists n_0$ such that $\forall n > n_0$, $k \leq np \leq K$ for some constants $k, K > 1$. Write $c = np$ and define $t \in (0,1)$ by $te^{-t} = ce^{-c}$. Then whp*

$$q_{\mathcal{PF}}(G_n) \geq \frac{2}{c} - \frac{t(2-t)}{c^2} + o(1).$$

Notice if we have $np \to c$ for $c > 1$ as in Theorem 6.2.15 then we can set $k = c - (c-1)/2$ and $K = c + 1$ to satisfy the conditions of Lemma 6.2.16. Hence it is enough for us to prove Lemma 6.2.16. We will use the greater generality of Lemma 6.2.16 in the proof of Theorem 6.1.5.

Proof. (of Lemma 6.2.16). We first work out the likely excess of the giant component of G_n, call this component H. By Lemma 6.7.5 whp $\ell(H) = (1 - t/c)(c + t - 2)/2$. Recall also that $m = cn(1 + o(1))/2$ by Lemma 6.2.8. Therefore the ratio of the excess in the giant component to the total number of edges in the graph is

$$\frac{\ell}{m} = 1 - \frac{2}{c} + \frac{t(2-c)}{c^2} + o(1). \tag{6.16}$$

By Lemma 6.2.13 whp the maximum degree, $\Delta(G_n) = O(\frac{\log n}{\log\log n})$. Hence it is easy to check that whp $2d < 2\sqrt{2dm} < 2|H| - d - 2 \leq 2e(H) - d$. Thus by Lemma 3.2.2, letting $h = e(H)$ be the number of edges in the giant,

$$q_{\mathcal{PF}}(H, m) \geq \frac{h}{m} - \frac{\ell}{m} - \frac{2h\sqrt{2\Delta}}{m^{3/2}}.$$

The term, $\frac{2h\sqrt{2d}}{m^{3/2}}$ is very small. Note that $h \leq m$ and $d = o(\log n)$ and so $\frac{2h\sqrt{2d}}{m^{3/2}} = o(1)$. We can substitute our bound on the likely excess from (6.16) and whp,

$$q_{\mathcal{PF}}(H, m) - \frac{h}{m} \quad \geq \quad -\frac{\ell}{m} + o(1) = -1 + \frac{2}{c} - \frac{t(2-c)}{c^2} + o(1). \tag{6.17}$$

Now extend this partition of H to a partition of G_n, by taking the vertex sets of the connected components in $G_n \backslash H$. Thus all edges in $G_n \backslash H$ will fall within parts, i.e.

$$q^E_{\mathcal{PF}}(G \backslash H, m) = 1 - \frac{h}{m}. \tag{6.18}$$

Also, whp each of the connected components in $G_n \backslash H$ is of size $O(\log n)$ and either a tree or unicyclic, and so the sum of squares of the degree sums of these parts will be $O((\log n)^2/n) = o(1)$. We can now calculate the lower bound for the prune-to-forest partition of G_n. By (6.17), (6.18) and our note on the degree sums of $G \backslash H$, whp

$$q_{\mathcal{PF}}(G_n) = q_{\mathcal{PF}}(H, m) + q^E_{\mathcal{PF}}(G \backslash H, m) + o(1) = \frac{2}{c} - \frac{t(2-c)}{c^2} + o(1).$$

□

6.3 Structure of an optimal partition

In the lower window, an interesting transition takes place as stated in Theorem 6.1.5. We illustrate this in Figure 6.9. Shown in the upper diagram, for $p = c/n$ and c fixed the connected components partition is whp optimal when $c < 1$ and whp not optimal when $c \geq 1$. The lower diagram illustrates the following, in the critical window with $np = 1 - \gamma$ where $\gamma = o(1)$ and $\gamma = n^{-\alpha}$ for some fixed $\alpha > 0$ then the connected components partition is whp optimal for $0 < \alpha < 1/4$ and whp not optimal for $\alpha \geq 1/4$.

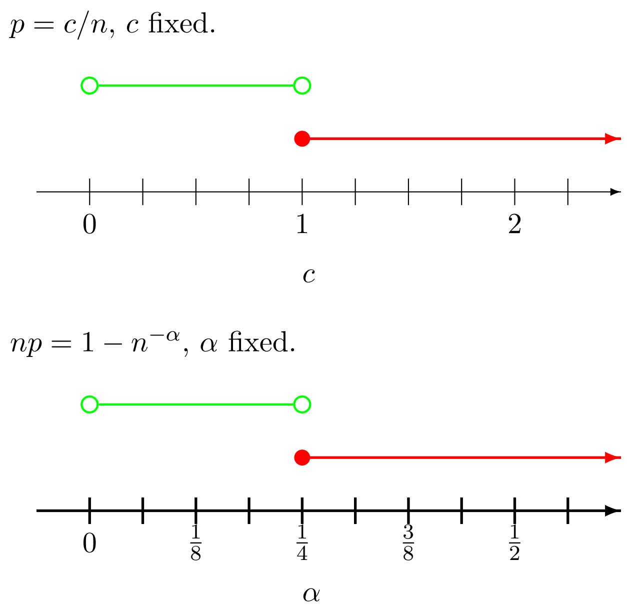


Figure 6.9: Diagrams to illustrate Theorem 6.1.5. They depict for which p the connected components partition is whp optimal (in green) and for which p there is whp a better partition (in red).

Now we restate Theorem 6.1.5 and provide a proof. Notice that $\gamma^- > \gamma^+$ and both γ^- and γ^+ are $n^{-1/4+o(1)}$.

Theorem 6.1.5 (restatement) *Define* $\gamma^- = \frac{(\log n)^{1/2}}{3n^{1/4}}$ *and* $\gamma^+ = \frac{(\log n)^{1/4}}{n^{1/4}}$. *If* $n^2 p \to \infty$ *and* $np \leq 1 - \gamma^-$ *then whp the connected components partition is the unique optimal partition. If* $np \geq 1 - \gamma^+$ *and* $np = O(1)$ *then whp there is a partition with higher modularity than the connected components partition.*

Proof. (of Theorem 6.1.5) The proof is in two parts. In **part 1**, we prove that the connected components partition is whp the unique optimal partition in the stated range. By Lemma 1.6.7, in a graph G with m edges if a connected component has less than $\sqrt{2m}$ edges then it is not cut in any optimal partition G. Hence to show the connected components partition is whp the unique optimal partition it suffices to show that whp all connected components have less than $\sqrt{2m}$ edges. Separate arguments are needed for three different ranges of p. First we attack the lower window.

Part 1, Range 1: $np = 1 + o(1)$ **and** $np \leq 1 - \gamma^-$**.**
For any p such that $np = 1-\gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$, by Lemmas 6.1.3 and 6.7.2 if we let L denote the vertex set in the connected component with the most edges then whp,

$$e(L) = \frac{1}{2\gamma^2}\log(\gamma^3 n)(1 + o(1)). \tag{6.19}$$

Thus it suffices to show that for $\gamma > \gamma^-$, whp $e(L) < \sqrt{2m}$. Recall that by Lemma 6.2.8, in this range, $m = (1-\gamma)n(1 + o(1))/2$ and so it is enough to show that for some $\epsilon > 0$

$$\log(\gamma^3 n) < 2\sqrt{2}(1-\varepsilon)\gamma^2\sqrt{n},$$

which is easily seen to be true for $\gamma > \gamma^-$.

Part 1, Range 2: $n^{7/4}p \to \infty$ **and** $np \leq 1 - \frac{1}{\log n}$**.**
This range is easy. For such p by Lemma 6.2.8, whp $m \geq n^2 p(1 + o(1))/2 \geq n^{1/4}$. By Lemma 6.7.1 and line (6.19) above whp any connected component has $O\big((\log n)^3\big)$ edges. Clearly $O\big((\log n)^3\big) < \sqrt{2n^{1/4}}$ and so we are done.

Part 1, Range 3: $n^2 p \to \infty$ **and** $n^{3/2}p \to 0$**.**
As in the proof of Lemma 6.2.1(i), for p in this range, whp G_n consists of disjoint edges (this follows from Lemma 6.2.2) and by Corollary 1.4.2 for a graph with disjoint edges the unique optimal partition is the connected components partition.

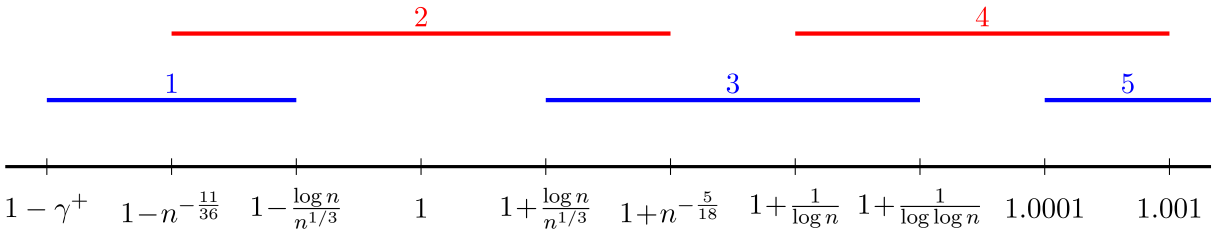


Figure 6.10: The five ranges in part 2 of the proof for Theorem 6.1.5 (not to scale).

Part 2

In part 2 we prove that the connected components partition is whp not optimal for a random graph G_n in the stated range of p. By Lemma 3.3.1 it is sufficient to show that whp G_n has a connected component H with maximal degree Δ, a set $E' \subseteq E(H)$ such that $H \backslash E'$ has treewidth t and which satisfies

$$e(H)^2 > |E'|m + 2e(H)\sqrt{(t+1)\Delta m} \tag{6.20}$$

In particular, if we take E' such that $H \backslash E'$ is a tree (of treewidth 1) then $|E'| + 1$ is precisely the excess, $\ell(H)$, of H. Therefore it suffices to show whp our graph has a connected component H such that

$$e(H)^2 > \ell(H)m + 2e(H)\sqrt{2\Delta m} \tag{6.21}$$

To argue this we split into five ranges of p. Figure 6.10 indicates a subset of the p covered by each range.

Part 2, Range 1: $np = 1-\gamma$ **where** $\gamma^3 n \to \infty$ **and** $\gamma < \gamma^+$**.**

Let L be the connected component of G_n with the largest number of edges. By Lemma 6.7.1 whp each connected component is either a tree or unicyclic. Hence whp L has treewidth 1 or 2. Thus, by (6.20) and taking $E' = \varnothing$, it suffices to show that whp $e(L) > 2\sqrt{3\Delta m}$. The maximum degree of L is whp less than $\log n$ by Lemma 6.2.13. Hence, recalling the likely number of edges in L from (6.19), it will be enough to show that for $\gamma \leq \gamma^+$ the following holds,

$$\log(\gamma^3 n) > 4\sqrt{6}\gamma^2\sqrt{n \log n}$$

which is clearly true and so range 1 is established.

Part 2, Range 2: $1 - n^{-11/36} \le np \le 1 + n^{-5/18}$**.**
Let $H = H(G_n)$ be the connected component with the maximal number of vertices. It is sufficient to prove H satisfies (6.21). Note that to show (6.21) is satisfied it is enough to show

$$\ell(G)m = o(e(H)^2) \text{ and } \sqrt{\Delta m} = o(e(H)). \tag{6.22}$$

Collate some results which hold whp for our random graph G_n and component H. By Corollary 6.7.8, as $np \le 1 + n^{-5/18}$, whp the excess of G_n is $O\big((n^{-5/18})^3 n\big) = O(n^{1/6})$. Also in this range, whp $m = O(n^2 p) = O(n)$ by Lemma 6.2.8. Together these results imply

$$\ell(H)m = O(n^{7/6}). \tag{6.23}$$

To bound $\sqrt{\Delta m}$ recall whp $\Delta = o(\log n)$ by Lemma 6.2.13 and so

$$\sqrt{\Delta m} = o(n^{1/2} \log n). \tag{6.24}$$

We can use line (6.19) to get a lower bound for $|H|$. For $np \ge 1 - n^{-11/36}$ whp

$$|H| \ge n^{11/18} (\log n)^2,$$

and hence whp,

$$e(H) \ge |H| - 1 \ge n^{11/18}. \tag{6.25}$$

Now we are effectively done. Comparing the lower bound in (6.25) to the upper bounds in (6.23) and (6.24) respectively shows that the two inequalities in (6.22) hold whp which completes the proof.

Part 2, Range 3: $np = 1 + \gamma$ **where** $\gamma = o(1)$ **and** $\gamma^3 n \to \infty$**.**
By taking Corollaries 6.7.7 and 6.7.8 together whp G_n has a connected component H with $e(H) = 2\gamma n(1 + o(1))$ and excess $\ell(H) = O(\gamma^3 n)$. As in range 2, whp $m = n(1 + o(1))/2$ and whp $\Delta = O(\log n)$. The RHS of (6.21) is whp

$$\ell(H)m + 2e(H)\sqrt{2\Delta m} = O(\gamma^3 n^2) + O(\gamma n \sqrt{n \log n}), \tag{6.26}$$

which compares to a LHS of $\Theta(\gamma^2 n^2)$. We show both terms in (6.26) are small. For the first term $\gamma = o(1)$ implies $\gamma^3 n^2 = o(\gamma^2 n^2)$. For the second term notice $\gamma n \sqrt{n \log n} = o(\gamma^2 n^2)$ is equivalent to $\sqrt{\frac{\log n}{n}} = o(\gamma)$. But $\gamma^3 n \to \infty$ implies $\gamma \gg n^{-1/3}$ and so the second term is also $o(\gamma^2 n^2)$. Thus whp there is such an H which is split in any optimal partition. This completes range 3.

Part 2, Range 4: $1 + \frac{1}{\log n} < np < 1.001$.
Whp G_n has a unique giant component by Lemma 6.1.2. The proof proceeds by showing whp this giant component, call it H, satisfies (6.21). More precisely we calculate the likely value of $e(H)^2 - \ell(H)m$ and then show it is whp larger than $2e(H)\sqrt{2\Delta m}$ where Δ is the maximum degree of G_n.

Write $c = np$ and define $t \in (0,1)$ by $te^{-t} = ce^{-c}$. Also write $b = 1 - t/c$. We first observe that for this range of p we have $0.99 < t < 1$. The upper bound is clear by definition. Now consider the function $y = xe^{-x}$. Note $y' = (1-x)e^{-x}$ and so y is decreasing for $x > 1$ and increasing for $x < 1$. Therefore $1 < c < 1.001$ implies $ce^{-c} > 1.001e^{-1.001} > 0.36787$. Similarly for $t \leq 0.99$, we have $te^{-t} \leq 0.99e^{-0.99} \leq 0.36787$ and hence $t > 0.99$ as required.

Now we analyse the expression $e(H)^2 - \ell(H)m$. By Lemma 6.7.5 whp $e(H) = bn(c+t)(1+o(1))/2$, $\ell(H) = bn(c+t-2)(1+o(1))/2$ and by Lemma 6.2.8 whp $m = cn(1+o(1))/2$. We write the error terms explicitly as the calculation is a little delicate,

$$e(H)^2 - \ell(H)m = \frac{1}{4}b^2n^2(c+t)^2 - \frac{1}{4}bcn^2(c+t-2) + o(b^2n^2(c+t)^2) + o(bcn^2(c+t-2)).$$

Many parts of the first two terms cancel. Substitute one instance of b in both the first and third terms by $b = 1 - t/c$. We can also simplify the error terms. As $1 < c < 1.001$ and $0.99 < t < 1$, we have $c, t = \Theta(1)$. Hence whp,

$$e(H)^2 - \ell(H)m = \frac{bn^2}{4}\left(2c - t^2 - \frac{t^3}{c}\right) + o(bn^2(1 - t/c)) + o(bn^2(c+t-2)). \tag{6.27}$$

Claim: that whp

$$e(H)^2 - \ell(H)m = \frac{bn^2}{4}\left(2c - t^2 - \frac{t^3}{c}\right)(1 + o(1)), \tag{6.28}$$

i.e. that the error terms in (6.27) behave nicely. We now show that the claim implies the result before returning to a proof of the claim. To establish that whp H satisfies (6.21) it is enough to prove that whp (6.28) is larger than $2e(H)\sqrt{2\Delta m}$. Recall by Lemmas 6.2.13 and 6.2.8 that whp $\Delta = o(\log n)$ and $m = \Theta(nc) = \Theta(n)$ and thus whp

$$2e(H)\sqrt{2\Delta m} = o(bn(c+t)\sqrt{n\log n}) = o(b\sqrt{n^3\log n}). \tag{6.29}$$

Comparing (6.28) and (6.29) it thus suffices to show that

$$2c - t^2 - \frac{t^3}{c} > \sqrt{\frac{\log n}{n}}. \tag{6.30}$$

We find a lower bound for the LHS of (6.30). The first equality below follows because $t < 1$ and the second because $c - 1/c > 0$,

$$2c - t^2 - \frac{t^3}{c} > 2c - 1 - \frac{1}{c} > c - 1 > \frac{1}{\log n}, \tag{6.31}$$

and so the inequality in (6.30) holds whp as required. Hence we have established the result for this range modulo the **claim** (6.28) which we now prove. Refer to (6.27) and note to prove the claim is it enough to prove the two inequalities below.

$$2c - t^2 - \frac{t^3}{c} \geq 1 - \frac{t}{c} \text{ and } 2c - t^2 - \frac{t^3}{c} \geq c + t - 2. \tag{6.32}$$

We can write $c = 1 + x$ and $t = 1 - y$ where $\frac{1}{\log n} < x < 0.001$ and $0 < y < 0.01$. Note $(1 + x)^{-1} \leq 1$ and so

$$\begin{aligned} 2c - t^2 - \frac{t^3}{c} &\geq 2(1 + x) - (1 - y)^2 - (1 - y)^3 \\ &= 2x + 5y - 3y^2 + y^3 \\ &\geq 2x + 4y \end{aligned}$$

Now we can see directly that (6.32) holds. For the first part,

$$1 - \frac{t}{c} \leq 1 - (1 - y)(1 - x) \leq x + y < 2c - t^2 - \frac{t^3}{c},$$

and for the second part,

$$c + t - 2 = x + y < 2c - t^2 - \frac{t^3}{c}.$$

Hence the claim is established which finishes the proof for this range.

Part 2, Range 5: $1.0001 < np < K$ **for some constant** $K > 1$**.**
Write $c = np$ and let $t \in (0, 1)$ be the solution to $te^{-t} = ce^{-c}$, then by Lemma 6.2.10, whp

$$q_{\mathcal{CC}}(G_n) = \frac{2t^2}{c^2} - \frac{t^4}{c^4} + o(1),$$

and by Lemma 6.2.16, whp

$$q_{\mathcal{PF}}(G_n) \geq \frac{2}{c} - \frac{t(2 - t)}{c^2} + o(1).$$

We **claim**, that whp $q_{\mathcal{PF}}(G_n) > q_{\mathcal{CC}}(G_n)$. To see this, noting our bounds above whp

$$q_{\mathcal{PF}}(G_n) - q_{\mathcal{CC}}(G_n) \geq \frac{2}{c} - \frac{2t}{c^2} - \frac{t^2}{c^2} + \frac{t^4}{c^4} + o(1) = \frac{1}{c^2}\left(2c - t^2\right)\left(1 - \frac{t}{c}\right) + o(1). \qquad (6.33)$$

The result follows by noting that $t < 1$ and $c > 1.0001$ together imply the RHS of (6.33) is strictly greater than 0. Hence whp the connected components partition is not optimal in this range. This concludes the argument for the final range and hence the proof is finished. □

6.4 Diminishing modularity at a constant factor past criticality

To prove that whp $q^*(G_n) = o(1)$ for $np \to \infty$, which we do in Lemma 6.4.5, requires us to compile both deterministic results on the modularity of graphs with certain properties in Section 6.4.1 and results concerning random graphs in Section 6.4.2 before proceding to the proof in Section 6.4.3.

6.4.1 Lemmas on modularity

The following lemma tells us in a sense that homogeneity implies low modularity. In particular if the number of edges within each part and the number of edges leaving each part are both approximately what we expect then our modularity is very small. We make this idea of homogeniety explicit by defining a notion of natural sets.

Definition 6.4.1. *We say a vertex subset A of graph G is* (α, β, p)-natural *if $A \neq \varnothing$ and*

$$\binom{|A|}{2} p(1-\alpha) \leq e(A) \leq \binom{|A|}{2} p(1+\alpha)$$

and

$$|A|(n-|A|)p(1-\beta) \leq e(A, V \backslash A) \leq |A|(n-|A|)p(1+\beta).$$

If we have a graph G with partition $\mathcal{A}$ in which every $A \in \mathcal{A}$ is a (α, β, p)-natural set then we can prove an upper bound on the modularity $q_{\mathcal{A}}(G)$ in terms of α, β and the number of edges in G.

Lemma 6.4.1. *Let $p > 0$ and $0 \leq \alpha, \beta, \delta < 1/4$. Suppose G is a graph on m edges with*

$$\binom{n}{2} p(1-\delta) \leq m \leq \binom{n}{2} p(1+\delta),$$

and $\mathcal{A}$ a vertex partition of G such that each $A \in \mathcal{A}$ is (α, β, p)-natural. Then

$$q_{\mathcal{A}}(G) \leq 3\alpha + 2\beta + 4\delta.$$

Proof. Fix a partition $\mathcal{A} = \{A_1, \ldots, A_k\}$ satisfying the conditions of the lemma and write $u_i = |A_i|/n$. This allows us to bound the edge contribution -

$$q^E_{\mathcal{A}}(G) \leq \frac{\sum_i \binom{u_i n}{2} p(1+\alpha)}{\binom{n}{2} p(1-\delta)} \leq \frac{1+\alpha}{1-\delta} \sum_i u_i^2.$$

We simplify this a bit. Note that $\delta < 1/3$ implies $(1-\delta)^{-1} < 1 + 3\delta/2$. Also, $\alpha < 1/3$ implies $(1+\alpha)(1+3\delta/2) < 1+\alpha+2\delta$. Hence

$$q_{\mathcal{A}}^{E}(G) \leq (1+\alpha+2\delta)\sum_i u_i^2. \tag{6.34}$$

Similarly, we can bound the degree tax. First observe that the sum of the degrees in a part is twice the number of internal edges plus the number of edges with between the part and the rest of the graph. Thus the degree sum of part A_i is bounded by

$$\mathrm{ds}(A_i) = 2e(A_i) + e(A_i, V\backslash A_i) \geq 2\binom{u_i n}{2}p(1-\alpha) + u_i(1-u_i)n^2 p(1-\beta),$$

which implies,

$$\mathrm{ds}(A_i) \geq n(n-1)pu_i\Big(1-\alpha-\beta\Big).$$

And hence we can calculate a lower bound on the contribution of one part, A_i, to the degree tax in terms of its size u_i and the parameters α, β, δ.

$$\begin{aligned}
\frac{1}{4m^2}\mathrm{ds}(A_i)^2 &\geq \frac{1}{(n(n-1)p(1+\delta))^2}\Big(n(n-1)pu_i\big(1-\alpha-\beta\big)\Big)^2. \\
&= \frac{u_i^2\Big(1-\alpha-\beta\Big)^2}{(1+\delta)^2} \\
&\geq u_i^2\Big(1-2\alpha-2\beta-2\delta\Big). \qquad (6.35)
\end{aligned}$$

We are now ready to provide an upper bound on modularity. Notice taking the sum over i of line (6.35) is a lower bound on the degree tax and line (6.34) provides an upper bound on the edge contribution. Hence,

$$q_{\mathcal{A}}(G) \leq \Big(3\alpha+2\beta+4\delta\Big)\sum_i u_i^2$$

Notice that $\sum_i u_i^2 \leq 1$ and so we are done. □

6.4.2 Lemmas concerning random graphs

We work with an Erdős-Rényi random graph with edge probability at least c/n for some constant $c > 1$. In Lemma 6.4.2 we show it is likely that for all sets of vertices which are not too small, the number of internal edges is not too big and the number of edges leaving is close to the expected value. This lemma will help us prove Lemma 6.4.3, a useful result to examine the likely modularity of G_n.

Lemma 6.4.2. *Fix $\eta > 0, 0 < \alpha, \beta < 1/4$ and constant c such that $c > \max\{\frac{5\log(1/\eta)}{\eta\alpha^2}, \frac{5}{2\beta^2}\}$. Suppose $np > c$ and let G_n be a random graph from $\mathcal{G}(n,p)$. Then whp the following two statements hold.*
(i) All vertex subsets A such that $|A| \geq \eta n$ satisfy

$$p\binom{|A|}{2}(1-\alpha) \leq e(A) \leq p\binom{|A|}{2}(1+\alpha).$$

(ii) All vertex subsets A satisfy

$$p|A|(n-|A|)(1-\beta) \leq e(A, V\backslash A) \leq p|A|(n-|A|)(1+\beta).$$

We now present an implication of this lemma on which the proof of Lemma 6.4.5 will hinge. The proof of Lemma 6.4.2 then appears at the end of this section. The lemma below is a bit technical but will allow us to show we can group together some of the smaller parts occuring in an optimal partition with negligible decrease in the modularity.

Lemma 6.4.3. *Let η, α, β, p satisfy the conditions of Lemma 6.4.2 and let G_n be a random graph from $\mathcal{G}(n,p)$.Suppose $\mathcal{A} = \{A_1, \ldots, A_k\}$ is a vertex partition with parts labeled in order of decreasing size, and j the largest index such that $|A_j| \geq \eta n$. Let $\mathcal{B} = \{B_1, \ldots B_h, R\}$ be a vertex partition such that $B_i = A_i$ for $i \leq j$, $\eta n \leq |B_i| < 2\eta n$ for $j < i \leq h$, $|R| < \eta n$ and $\mathcal{A}$ refines $\mathcal{B}$. Then whp for any such $\mathcal{A}, \mathcal{B}$, $q_{\mathcal{A}}(G_n) - q_{\mathcal{B}}(G_n) < 3\eta/2$.*

Proof. We want to bound the possible decrease in modularity caused by the change in the partition from $\mathcal{A}$ to $\mathcal{B}$. Notice the edge contribution of $\mathcal{B}$ will be at least that of $\mathcal{A}$ so we can bound the decrease in terms of the degree tax, i.e. $q_{\mathcal{A}}(G_n) - q_{\mathcal{B}}(G_n) \leq q^D_{\mathcal{B}}(G_n) - q^D_{\mathcal{A}}(G_n)$. We can simplify this expression further

$$\begin{aligned} q^D_{\mathcal{B}}(G_n) - q^D_{\mathcal{A}}(G_n) &= \frac{1}{4m^2}\Big(\sum_{i>j}\mathrm{ds}(B_i)^2 + \mathrm{ds}(R)^2 - \sum_{i>j}\mathrm{ds}(A_i)^2\Big) \\ &\leq \frac{1}{4m^2}\Big(\sum_{i>j}\mathrm{ds}(B_i)^2 + \mathrm{ds}(R)^2\Big). \end{aligned}$$

By Lemma 6.4.2, as $|B_i|, |R| < 2\eta n$ for $i > j$ whp we can bound $\text{ds}(B_i)$ and $\text{ds}(R)$ by bounding the sum of twice the number of internal edges and the number of edges leaving

$$2\binom{2\eta n}{2}p(1+\alpha) + 2\eta(1-2\eta)n^2p(1+\beta) \quad \leq \quad 2\eta(1+\beta+\alpha\eta-2\beta\eta)n^2p$$

Note that $0 \leq x_i \leq t$ and $\sum_i x_i \leq 2m$ together imply that $\frac{1}{4m^2}\sum_i x_i^2 \leq t/2m$. Also recall we can take $\gamma = n^{-1/2}\log n$ and by Lemma 6.2.8 whp

$$e(G) > \binom{n}{2}p(1-\gamma) = n^2p(1-\gamma)(1-1/n)/2 = n^2p(1+o(1))/2$$

and thus whp,

$$\begin{aligned} q_{\mathcal{A}}(G_n) - q_{\mathcal{B}}(G_n) &\leq \frac{2\eta(1+\beta+\alpha\eta-2\beta\eta)n^2p}{2\binom{n}{2}p(1-\gamma)} \\ &= 2\eta(1+\beta+\alpha\eta-2\beta\eta)(1+o(1)) \\ &< 3\eta/2 \end{aligned}$$

and we are done. □

To prove Lemma 6.4.2 we need a concentration result. The following version of Chernoff appears as parts (b) and (c) of Theorem 2.3 in the survey on concentration by McDiarmid [45].

Lemma 6.4.4 (Chernoff). *Let the random variables $X_1, X_2, \ldots, X_n$ be independent with $|X_i| \leq 1$, $\forall i$ and denote $S_n = \sum_k X_k$ and $\mu = \mathbb{E}(S_n)$. Then for all $\delta > 0$,*

$$\begin{aligned} \mathbb{P}(S_n \geq (1+\delta)\mu) &\leq \exp(-\delta^2\mu/(2(1+\delta/3))) \\ &\leq \exp(-\delta^2\mu/3) \quad \textit{for } 0 \leq \delta \leq 1. \\ \mathbb{P}(S_n \leq (1-\delta)\mu) &\leq \exp(-\delta^2\mu/2). \end{aligned}$$

Proof. (of Lemma 6.4.2) We use Chernoff, Lemma 6.4.4, to show that for a fixed set of vertices the probabilities p_1 of having a large number of internal edges or p_2 of having a number of edges to the rest of the graph that varies too much from the expected are both small. Fix $|A| = an$, and recall $|A| \geq \eta n$.

Let p_1 and p_2 describe the probability that a fixed set of vertices $|A| = a$ will not satisfy the internal edge or external edge condition respectively.

$$
\begin{aligned}
p_1(a) = \mathbb{P}\left(\left| \frac{e(A)}{\binom{|A|}{2} p} - 1 \right| > \alpha \right) &\leq 2 \exp\left(- \frac{\alpha^2 \mathbb{E}(e(A))}{2(1+\alpha/3)} \right) \\
&= 2 \exp\left(- \frac{\alpha^2 |A|(|A|-1)p}{4(1+\alpha/3)} \right) \\
&= 2 \exp\left(- \frac{\alpha^2 a^2 nc}{4(1+\alpha/3)} + \frac{\alpha^2 ac}{4(1+\alpha/3)} \right)
\end{aligned}
$$

The number of ways of picking a vertex subset is less than 2^n. Note $\sum_{an=1}^{n} p_2(a) \leq 2^n p_2(1/2)$ and for $c > 5/(2\beta^2)$, $2^n p_2(1/2) \to 0$. To bound the internal edge condition is a little trickier but likewise starts with an application of Chernoff's inequality.

$$
\begin{aligned}
p_2(a) = \mathbb{P}\left(\left| \frac{e(A, V \backslash A)}{p|A|(n-|A|)} - 1 \right| > \beta \right) &\leq 2 \exp\left(- \frac{\beta^2 \mathbb{E}(e(A, V\backslash A))}{2} \right) \\
&= 2 \exp\left(- \frac{\beta^2 |A|(n-|A|)p}{2} \right) \\
&\leq 2 \exp\left(- \frac{\beta^2 a(1-a)nc}{2} \right)
\end{aligned}
$$

The expected number of sets A which will not satisfy the internal edge condition can be bounded by (using $\binom{n}{an} \leq (e/a)^{an}$)

$$
\sum_{an=\eta n}^{n} \binom{n}{an} \exp\left(- \frac{\alpha^2 a^2 cn}{4(1+\alpha/3) + O(1)} \right)
$$
$$
\leq (1-2\eta) n \exp\left(- an\Big(\frac{\alpha^2 ac}{4(1+\alpha/3)} - \log(1/a) - 1 \Big) + O(1) \right)
$$

Thus for $c > \frac{5 \log(1/\eta)}{\eta \alpha^2}$ the expected number of sets violating the edge condition tends to 0, i.e. whp all sets satisfy the internal edge condition. □

6.4.3 The proof

In this section we prove that for $np \geq c$, for large constant c, the likely maximum modularity of the random graph is bounded above by a function in c.

Lemma 6.4.5. *Suppose G_n is a random graph from $\mathcal{G}(n,p)$. Fix $0 < \varepsilon < 1/80$. Then $\exists c_0$ such that if $np > c_0$ then whp $q^*(G_n) < \varepsilon$ and we may take $c_0 = 2^{14}\varepsilon^{-3}\log(1/\varepsilon)$.*

Proof. Fix $\varepsilon > 0$ and let $c_0 = 2^{14}\varepsilon^{-3}\log(1/\varepsilon)$. Set $\alpha = 3\varepsilon/4$, $\beta = \eta = \varepsilon/40$, $\delta = \varepsilon/300$ and note that $3\alpha + 2\beta + 7\eta + 14\delta < \varepsilon$. Also note that by our choice of c_0, α, β, η that $c_0 > \max\{\frac{5\log\eta}{\alpha^2\eta}, \frac{5}{2\beta^2}\}$. Hence by Lemma 6.4.2 whp G_n has the property that for all vertex subsets A with $|A| \geq \eta n$, it holds that A is (α, β, p)-natural.

Outline. We first show that any partition in which each part has at least ηn vertices has very low modularity. Then we show for an arbitrary partition $\mathcal{A}$ of G, there is a partition $\mathcal{C}$ of G' of this form such that the difference in their respective modularities is small. We do this in two steps. First we show we can group all parts in $\mathcal{A}$ with size less than ηn into sets with size in the interval $[\eta n, 2\eta n]$ with a small exception set R. This changes the modularity very little. We can then delete the vertices in the exception set with little change in modularity to yield a partition $\mathcal{C}$ of $G\backslash R$ in which all parts have at least ηn vetices. See Figure 6.11 for an ilustration.

Let $\mathcal{A}$ be a vertex partition which maximises the modularity, and is such that each part induces a connected graph. The existence of such a partition is guaranteed by Lemma 1.6.1. There are two cases: in the first case suppose $|A| \geq \eta n$ for each $A \in \mathcal{A}$. Hence whp each set $A \in \mathcal{A}$ is (α, β, p)-natural. Write $m = e(G)$, by Lemma 6.2.8 whp $m = \binom{n}{2}(1 + o(1))$. These together imply, by Lemma 6.4.1, whp $q_{\mathcal{A}}(G) \leq 3\alpha + 2\beta + o(1) < \varepsilon$ and we would be done. So we suppose not.

Step 1, we define $\mathcal{B}$. Relabel the sets in $\mathcal{A}$ in order of decreasing size and let j be the largest index such that $|A_j| \geq \eta n$. Let $\mathcal{B} = \{B_1, \dots B_h, R\}$ be a vertex partition such that $B_i = A_i$ for $i \leq j$, $\eta n \leq |B_i| < 2\eta n$ for $j < i \leq h$, $|R| < \eta n$ and $\mathcal{A}$ refines $\mathcal{B}$. The existence of such a partition can be seen by greedily taking unions of sets in $\mathcal{A}$ of size $< \eta n$ to make sets B_i of size $\eta n \leq |B_i| < 2\eta n$ until less than ηn vertices remain which we place in R. Now we bound the possible decrease in modularity caused by modifying the partition. By Lemma 6.4.3 and our choice of parameters whp

$$q_{\mathcal{A}}(G_n) - q_{\mathcal{B}}(G_n) \leq 3\eta/2. \tag{6.36}$$

Step 2, we define $\mathcal{C}$. Let $\mathcal{C}$ be the restriction of $\mathcal{B}$ to $G_n\backslash R$. Recall isolated vertices don't affect the modularity by Lemma 1.4.8. Thus the quantitiy $q_{\mathcal{C}}(G_n\backslash R)$ is exactly $q_{\mathcal{B}}(G')$ where G' is the graph with the edge sets $E(R)$ and $E(R, V\backslash R)$ removed.

We **claim** that whp $E(R) \leq 2(\delta+\eta^2)m$ and $E(R, V\backslash R) < (5\eta/2+2\delta)m$.

To prove the claim first observe by Lemma 6.2.8 whp $|m - \binom{n}{2}p| < \delta$. As $|R| < \eta n$ there exists $R' \subset V\backslash R$ such that $A = R \cup R'$ has size ηn. Hence whp this vertex set A is (α, β, p)-natural and thus whp

$$e(A) + e(A, V\backslash A) < \binom{\eta n}{2}p(1+\alpha) + \eta(1-\eta)n^2p(1+\beta) < 5\eta n^2 p/4 < (5\eta/2+2\delta)m.$$

Also note $E(R) \leq E(A)$ and hence $E(R) \leq \binom{\eta n}{2}p(1+\alpha) < 2(\delta+\eta^2)m$ and so we have proven the claim.

By the claim and Lemma 1.4.5 whp

$$q_{\mathcal{B}}(G_n) - q_{\mathcal{C}}(G_n\backslash R) < 6(\delta+\eta^2) + 2(5\eta/2+2\delta) < 11\eta/2 + 10\delta. \tag{6.37}$$

Step 3. By construction the set R was the only part in $\mathcal{B}$ containing fewer than ηn vertices. Hence after its removal our vertex partition $\mathcal{C}$ of $G_n\backslash R$ contains only parts with at least ηn vertices and by Lemma 6.4.1 whp

$$q_{\mathcal{C}}(G_n\backslash R) < 3\alpha + 2\beta + 4\delta. \tag{6.38}$$

Now we can add the inequalities (6.36), (6.37) and (6.38) to obtain

$$q_{\mathcal{A}}(G_n) < 3\alpha + 2\beta + 7\eta + 14\delta < \varepsilon$$

and the proof is complete. □

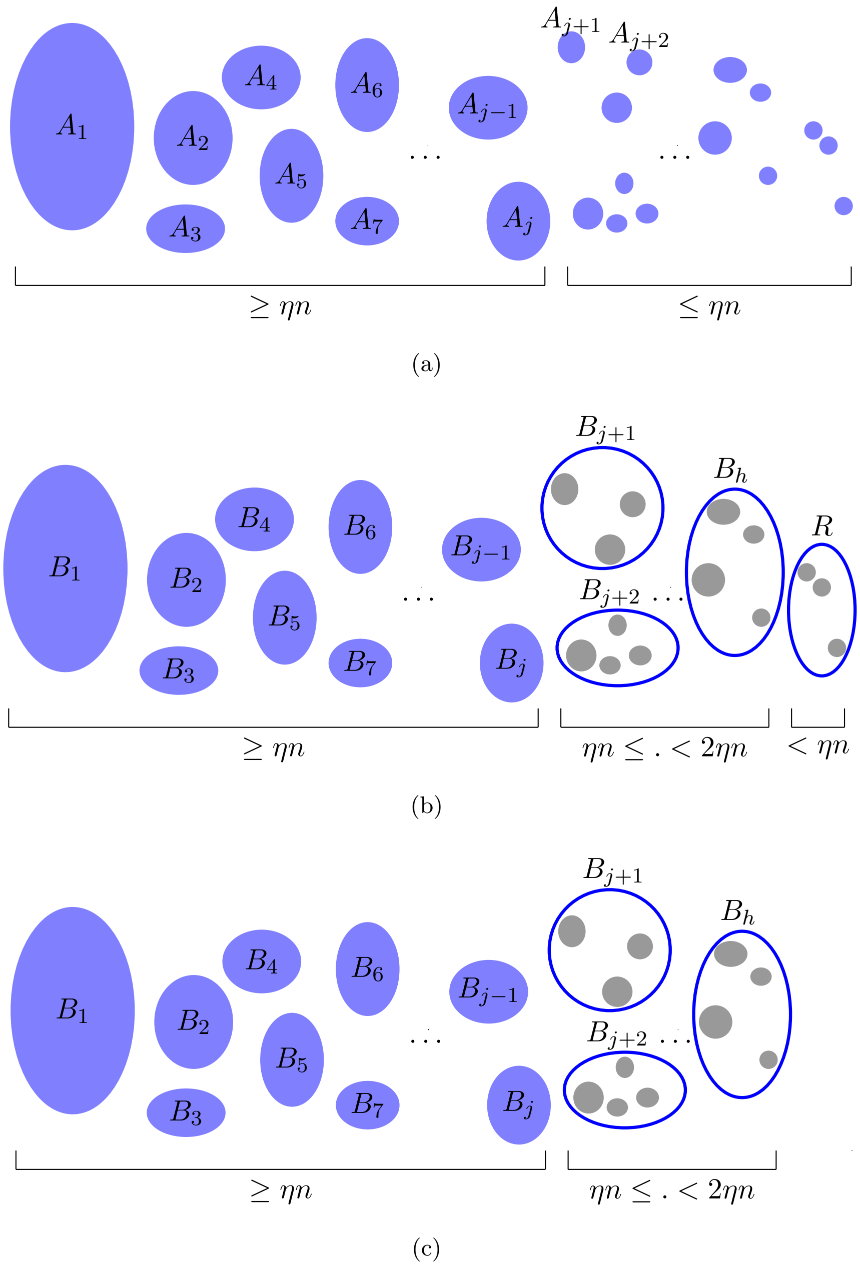


Figure 6.11: An illustration of the succesive partitions defined in the proof of Lemma 6.4.5.

6.5 Proof of the three phases

In this section we will prove Theorem 6.1.1 but first we need one more lemma.

Lemma 6.5.1. *Fix $c > 1$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. Then $\exists \varepsilon > 0$ such that if $np \to c$ then whp $q^*(G_n) < 1 - \varepsilon$.*

For the proof of this lemma we will need the following result concerning edge expansion in the giant component. In order to state it we define a (δ, η)-cut of $G = (V, E)$ to be a bipartition of V into V_1, V_2 such that both sets have at least $\delta|V|$ vertices and $e(V_1, V_2) < \eta|V|$. We will need only the case $\delta = 1/3$ but state the complete version for interest.

Lemma 6.5.2 (Luczak, McDiarmid, Lemma 2 [41])**.** *Let $np \to c$ for some constant $c > 1$ and suppose G_n is a random graph from $\mathcal{G}(n,p)$. For any $\delta > 0$, there exists $\eta > 0$ such that whp the giant component of G_n has no (δ, η)-cut.*

Proof. (of Lemma 6.5.1) First note that by Lemma 6.5.2, we can fix $\eta > 0$ such that whp there is no $(1/3, \eta)$-cut in the giant component H of G.

Define $t \in (0,1)$ to solve $te^{-t} = ce^{-c}$ and set $\varepsilon = \min\{\frac{(c-t)^2}{3c^4}, \frac{\eta(c-t)}{c^2}\}$. We will show that whp $q^*(G_n) < 1 - \varepsilon$.

By Lemma 6.1.2 whp there is a unique giant component H with $|H| = (1 - t/c)n(1 + o(1))$ and by Lemma 6.7.5 $e(H) = (1 - t/c)(c + t)(1 + o(1))/2$.

Let $\mathcal{A}$ be a partition of G_n with maximal modularity such for that each part the restriction of G_n to the vertices in that part is a connected graph. (The existence of such an $\mathcal{A}$ is guaranteed by Lemma 1.6.1.) This implies any part in $\mathcal{A}$ lies entirely within or entirely out of the giant component H. Let $\mathcal{A}_H = \{A \in \mathcal{A} : A \subseteq V(H)\}$. We will restrict our attention to $\mathcal{A}_H$. There are two cases to consider.

Case 1. Suppose there is some part, say $A_1 \in \mathcal{A}_H$ such that $|A_1| \geq |H|/3$. As A_1 is connected whp $\text{ds}(A_1) \geq 2(|A_1| - 1) \geq 2(1 - t/c)n(1 + o(1))/3$. By Lemma 6.2.8 $m = cn(1 + o(1))/2$. Together these allow us to construct a lower bound on the degree tax by considering the contribution from part A_1: whp,

$$q^D_{\mathcal{A}}(G_n) \geq \frac{1}{4m^2}\text{ds}(A_1)^2 \geq \frac{4(1 - t/c)^2 n^2}{9c^2 n^2}(1 + o(1)) > \frac{(c - t)^2}{3c^4}.$$

Case 2. Now suppose that $|A| < |H|/3$ for all $A \in \mathcal{A}_H$. By load balancing results we can divide the parts of $\mathcal{A}_H$ into two groups $\mathcal{A}_{H_1}, \mathcal{A}_{H_2}$ so that $\sum_{A\in\mathcal{A}_{H_1}} |A|$ and $\sum_{A\in\mathcal{A}_{H_2}} |A|$ are at least $|H|/3$ i.e. so that they each have at least a third of the vertices of our giant component H. Let $H_1 = \cup_{A\in\mathcal{A}_{H_1}} A$ and define H_2 similarly. Recall Lemma 6.5.2 tells us there is no $(1/3, \eta)$-cut. Hence whp $e(H_1, H_2) \geq \eta|H| = \eta(1 - t/c)n(1 + o(1))$.

Notice the edge contribution is one less the ratio of the number of edges which lie between parts to the total number of edges, i.e. $q^E_{\mathcal{A}}(G_n) = 1 - \frac{1}{2m}\sum_{A\neq A'\in\mathcal{A}} e(A, A')$. Each of the edges between H_1, H_2 lies between distinct parts in $\mathcal{A}$ and so we have placed an upper bound on the edge contribution. Thus whp,

$$q^E_{\mathcal{A}}(G_n) \leq 1 - \frac{1}{m}e(H_1, H_2) \leq 1 - \frac{2\eta(c-t)}{c^2}(1 + o(1)) < 1 - \frac{\eta(c-t)}{c^2},$$

and we are done. □

We can now prove Theorem 6.1.1 which identifies three phases of likely maximum modularity.

Proof. (of Theorem 6.1.1)
Part (i).
We want to show that for p in the range $n^2p \to \infty$ and $np \leq 1 + o(1)$ the random graph $G_n \sim \mathcal{G}(n, p)$ satisfies $q^*(G_n) \to 1$. First observe the maximum modularity is at least that achieved by the connected components partition: the vertex partition where each part is the vertex set of a connected component. That is, for any graph G and $\mathcal{CC} = \mathcal{CC}(G)$, $q^*(G) \geq q_{\mathcal{CC}}(G)$. Hence it suffices to show that whp $q_{\mathcal{CC}}(G_n) \to 1$ which we break into two overlapping ranges to prove.

Range 1: $n^2p \to \infty$ and $np \leq 1/2$. By part (iii) of Lemma 6.2.1 in this range whp

$$q_{\mathcal{CC}}(G_n) = 1 - \frac{1}{m(1-np)} + O\left(\frac{1}{m}\right) = 1 + o(1),$$

where the second equality holds because $n^2p \to \infty$ implies whp $m \to \infty$ by Lemma 6.2.8.

Range 2. $1/3 \leq np \leq 1+o(1)$**.** Let T be the maximum number of edges in any connected component of G_n. Then by Lemma 1.6.8, we get a lower bound $q_{\mathcal{CC}}(G_n) = 1 + O(T/m)$. Note the maximum number of edges in a connected component is a monotone property and so by Corollary 6.7.7 whp $T = o(n)$. Also by Lemma 6.2.8 whp $m = \Theta(n^2p) = \Theta(n)$ and thus whp $q_{\mathcal{CC}}(G_n) = 1 + O(T/m) = 1 + o(1)$.

Part (ii).

This statement ties together four results we have already proven. First by Lemma 6.5.1 there exists ε_1 such that whp $q^*(G_n) < 1 - \varepsilon_1$. Both lower bounds can be covered at the same time: by Theorem 6.2.11, whp $q^*(G_n) > \frac{1}{c+1}$ and so we can take $\varepsilon_2 = \frac{1}{c+1}$ and whp $q^*(G_n) > \varepsilon_2$ and let $\varepsilon = \min\{\varepsilon_1, \varepsilon_2\}$. It is enough to show that whp $q^*(G_n) < \frac{32 \log c}{c^{1/3}}$. This requires a little calculation. By Lemma 6.4.5 for any fixed $\alpha > 0$ if $np > \frac{2^{14}\log(1/\alpha)}{\alpha^3}$ then whp $q^*(G_n) < \alpha$. Now put $\alpha = \frac{32 \log c}{c^{1/3}}$, then we only need to check that $\frac{2^{14}\log(1/\alpha)}{\alpha^3} < c$. A simple calculation confirms this and completes the proof.

Part (iii).

We want to show that $np \to \infty$ implies $q^*(G_n) \to 0$. This follows from Lemma 6.4.5. Fix a small $\varepsilon > 0$. As $np \to \infty$, in particular for n large enough, $np > \frac{2^{14}\log(1/\varepsilon)}{\varepsilon^3}$, so by Lemma 6.4.5 whp $q^*(G_n) < \varepsilon$. Hence in this range, whp $q^*(G_n) = o(1)$ as claimed. □

There is one more theorem claimed in the introduction which we are yet to prove. The theorem in question is Theorem 6.1.4, stated on p98, which contains slightly more detailed results on the likely maximum modularity of a random graph than Theorem 6.1.1.

Proof. (of Theorem 6.1.4). The required bounds on $q^*(G_n)$ for both the range $np \to c$ for constant $c > 1$ and also the range $np \to \infty$ are proven in parts (ii) and (iii) respectively in the proof of Theorem 6.1.1. Hence it will be sufficient if we can prove the statement in italics.

If $n^2p \to \infty$ and $np \le c + o(1)$ for constant $c < 1$, then whp

$$q^*(G_n) = 1 - \Theta\left(\frac{1}{n^2p}\right),$$

and if $np = 1 + \gamma$ for $\gamma = o(1)$, then whp

$$q^*(G_n) = \begin{cases} 1 - O(\frac{1}{\gamma n}) & \text{if } \gamma^3 n \to -\infty \\ 1 - O\left(\frac{1}{n^{2/3}}\right) & \text{if } \gamma^3 n \to \lambda \in (-\infty, \infty) \\ 1 - O(\gamma^3) - O\left(\gamma\sqrt{\frac{\log n}{n \log\log n}}\right) & \text{if } \gamma^3 n \to \infty. \end{cases}$$

These four statements can be pieced together from earlier results in the chapter. First, define γ^- as in Theorem 6.1.5 and then this theorem implies if $n^2p \to \infty$ and $np \le 1 - \gamma^-$ whp the connected components partition is optimal. Hence in the first range whp $q^*(G_n) =$

range p		$1-q^*(G_n)$ whp ...		
$n^{-2} \ll p \ll n^{-1}$		$\sim \frac{1}{m}$	$\sim \frac{2}{n^2 p}$	
$\frac{1}{n^2} \ll p \leq \frac{c}{n}(1+o(1))$	$c<1$	$\Theta(\frac{1}{m})$	$\Theta(\frac{1}{n^2 p})$	
$p=\frac{1}{n}(1-\gamma)$	$\gamma > \gamma^-$	$\sim \frac{2}{\gamma m}$	$\sim \frac{4}{\gamma n}$	
$p=\frac{1}{n}(1-\gamma)$	$\gamma \leq \gamma^-$	$O(\frac{1}{\gamma m})$	$O(\frac{1}{\gamma n})$	~ 0
$p=\frac{1}{n}(1+\gamma)$	$\gamma^3 n = O(1)$	$O(\frac{1}{m^{2/3}})$	$O(\frac{1}{n^{2/3}})$	
$p=\frac{1}{n}(1+\gamma)$	$\gamma^3 n \to \infty$	$O(\gamma^3)+O(\gamma\sqrt{\frac{\log m}{m \log\log m}})$	$O(\gamma^3)+O(\gamma\sqrt{\frac{\log n}{n \log\log n}})$	
$p \sim \frac{c}{n}$	$c>1$	$1-\frac{1}{c+1} < * < 1-\frac{32\log c}{c^{1/3}}$	$1-\frac{1}{c+1} < * < 1-\frac{32\log c}{c^{1/3}}$	
$p \gg n$		~ 1	~ 1	~ 1

Figure 6.12: Table of asymptotic bounds which hold whp for $1-q^*(G_n)$.

$q_{\mathcal{CC}}(G_n)$. But $q_{\mathcal{CC}}(G_n) = \Theta(\frac{1}{n^2 p})$ by Lemma 6.2.1(iii) and so the first statement is established.

range p		$1-q^*(G_n)$ whp ...			
$n^{-2} \ll p \ll n^{-3/2}$		$* = \frac{1}{m}$			
$n^{-2} \ll p \ll n^{-1}$		$\frac{1}{m} \leq * \preceq \frac{1}{m}$	$\sim \frac{1}{m}$	$\sim \frac{2}{n^2 p}$	
$n^{-1} \ll p \ll cn^{-1}$	$c<1$	$\frac{1}{m} \leq * \preceq \frac{2}{mc}(\frac{1}{1-c}+2)$			
$p \sim \frac{c}{n}$	$c<1$	$\frac{2}{mc(1-c)} \preceq * \preceq \frac{2}{mc}(\frac{1}{1-c}+2)$	$\Theta(\frac{1}{m})$	$\Theta(\frac{1}{n^2 p})$	~ 0

Figure 6.13: Table of asymptotic bounds which hold whp for $1-q^*(G_n)$, results for small p.

The final three statements are only lower bounds on the modularity so it is enough to demonstrate a particular partition which meets that bound. In the lower window take the connected components partition. Then whp $q^*(G_n) \geq q_{\mathcal{CC}}(G_n) = 1 - O(\frac{1}{\gamma n})$ by Lemma 6.2.1(iv). For the central region of the critical window we also take the connected components partition. Then by Lemma 6.2.1(v) whp $q^*(G_n) = 1 - O(n^{-2/3})$ as required. Finally, for the upper window we take the prune-to-forest partition which is bounded in Theorem 6.2.14. Hence whp $q^*(G_n) \geq q_{\mathcal{PF}}(G_n) = O(\gamma^3) + O(\gamma\sqrt{\frac{\log n}{n \log\log n}})$. □

See Figures 6.12 and 6.13 for a summary of our best bounds on the likely maximum modularity for different ranges of p. Whenever $n^2 p \to \infty$ and $np \leq 1 - \gamma^-$ then Theorem 6.1.5 tells us whp the connected components partition is optimal so any results in this range are simply copied across from Figures 6.5 and 6.6.

6.6 Concentration and expectation of maximum modularity

In Theorem 6.6.1 we show that the maximum modularity of a random graph is highly concentrated about its expected value.

Theorem 6.6.1. *Suppose* $\exists n_0, c$ *such that* $\forall n > n_0,\ 1 < np < c$ *and let* $G_n \sim \mathcal{G}(n,p)$. *Then whp*

$$|q^*(G_n) - \mathbb{E}[q^*(G_n)]| < \frac{\log n}{n^{1/2}}.$$

The proof of this theorem uses Lemma 1.4.7 from earlier in the thesis, a robustness result where we bound the sensitivity of modularity to changes in the edge set adjacent with one vertex. We will also need a concentration result and use the following which appears as Theorem 3.7 in [45], extending on Theorem 3.1 in the same paper where there is no 'bad' set.

Lemma 6.6.2 (McDiarmid [45]). *Let* $\boldsymbol{X} = (X_1, X_2, \ldots, X_N)$ *be a family of independent random variables, with* X_i *taking values in a set* A_i *for each* i. *Furthermore let* $\boldsymbol{B}$ *be any 'bad' subset of* $\prod_{i=1}^N A_i$. *Suppose that for each* j *the function* $f : \prod_{i=1}^N A_i \to \mathbb{R}$ *satisfies* $|f(\boldsymbol{x}) - f(\boldsymbol{x}')| \leq c_j$ *whenever* $\boldsymbol{x}, \boldsymbol{x}' \in \prod_{i=1}^N A_i$ *differ only in the* j*-th component and* $\boldsymbol{x}, \boldsymbol{x}' \notin \boldsymbol{B}$. *Then, for any* $z > 0$,

$$\mathbb{P}\big(\big|f(\boldsymbol{X}) - \mathbb{E}(f(\boldsymbol{X}))\big| \geq z\big) \leq 2\exp\big(-2z^2/\textstyle\sum_{i=1}^N c_i^2\big) + \mathbb{P}\big(\boldsymbol{B}\big).$$

We are now ready to prove the theorem.

Proof. (of Theorem 6.6.1) We use a vertex exposure martingale. Write $m = e(G_n)$. Earlier, in Lemmas 6.2.8 and 6.2.13, we established that whp $\Delta(G_n) < 2\log n/(\log\log n)$ and whp $m < cn/3$, let $\boldsymbol{B}$ be the set of graphs which do not satisfy these inequalities. Furthermore, by Lemma 1.4.7, when the edges adjacent with one vertex are changed the difference in maximum modularity is less than $5\Delta/m$. Thus for $G, G' \notin \boldsymbol{B}$ the difference $|q^*(G) - q^*(G')|$ is less than $r = 30\log n/(cn\log\log n)$. Thus to show that the maximum modularity is whp within t of its expectation it is sufficient to show $2\exp(-2t^2/nr^2) \to 0$, equivalently that $t^2/nr^2 \to \infty$. Thus we can take $t = \log n/\sqrt{n}$ and we are done. □

For large n, we show that the expected maximum modularity of a random graph with edge probability p is similar to that of a random graph with edge probability p' when p' is near p. At the moment it is an open question whether the expected modularity $\mathbb{E}(q^*(G_{n,c/n}))$ tends to a limit $f(c)$ as $n \to \infty$. However if we could prove such a limit did exist then Theorem 6.6.3 would show that this limit $f(c)$ is continuous in c.

To state the following theorem we denote by $G_{n,c/n}$ the random graph $G_n \sim \mathcal{G}(n, c/n)$ and similarly by $G_{n,p}$ the random graph $G_n \sim \mathcal{G}(n, p)$.

Theorem 6.6.3. *$\forall c, \varepsilon > 0$, $\exists \delta > 0, N : \forall n > N$,*

$$np \in [c-\delta, c+\delta] \Rightarrow \Big|\mathbb{E}\big[q^*(G_{n,c/n}) - q^*(G_{n,p})\big]\Big| < \varepsilon.$$

We pause to prove a lemma that will be useful in the proof of Theorem 6.6.3.

Lemma 6.6.4. *Fix $\varepsilon > 0$, $c > 0$. Let $k \leq \binom{n}{2}$ be an integer and $X_1, \ldots, X_k$ be independent binomial random variables where $P(X_i = 1) = c/n \; \forall i$. Set $S = \sum_i X_i$. Then for all integers $n > \lceil \frac{16}{3c} \log(4/\varepsilon) \rceil$,*

$$\mathbb{P}(S \geq nc) < \varepsilon/2.$$

Proof. First observe that it suffices to prove this for $k = \binom{n}{2}$. By Chernoff, Lemma 6.4.4,

$$\mathbb{P}\Big(S \geq (1+\delta)(n-1)c/2\Big) \quad \leq \quad \exp\left(-\frac{\delta^2(n-1)c}{4(1+\delta/3)}\right)$$

Thus we want to determine N such that $\exp(-\frac{\delta^2 Nc}{4(1+\delta/3)}) < \varepsilon/2$ for $\delta = 1$, i.e. $\exp(-\frac{3Nc}{16}) < \varepsilon/2$. Hence we can choose $N = \lceil \frac{16}{3c} \log(2/\varepsilon) \rceil$ and $n \geq N+1$ will behave as required. $\square$

Proof. (of Theorem 6.6.3) Set $\delta = \varepsilon/16$, $N = \lceil \frac{16}{3c} \log(2/\varepsilon) \rceil$ and fix some integer $n > N$ and $c' \in [c-\delta, c+\delta]$. Write $c_0 = \min\{c, c'\}$ and $c_1 = \max\{c, c'\}$.

Recall that to sample an Erdős-Rényi random graph with edge probability p it is equivalent to pick each edge independently with probability $p' < p$ and then pick each of the remaining non-edges independently with probability $p'' = (p-p')/(1-p')$. We write this as

$$\mathbb{P}_p(G) = \sum_{G' : E(G') \subseteq E(G)} \mathbb{P}_{p'}(G')\mathbb{P}_{p' \to p}(G' \to G).$$

We will use this technique with $p = c_0/n$, $p' = c_1/n$, $p'' = (c_1 - c_0)/(n - c_1)$. Note that $c_1 - c_0 \leq \delta/n$ by assumption and so $p'' \leq 2\delta/n$. Hence by Lemma 6.6.4 as we choose remaining non-edges in G' fewer than $2\delta n$ edges are added with probability at least $1 - \varepsilon/2$. We are almost done.

$$\begin{aligned}\mathbb{E}\big[q^*(G_{n,c_1/n}))\big] &= \sum_G \mathbb{P}_{\frac{c_1}{n}}(G)q^*(G) \\ &= \sum_{G'} \mathbb{P}_{\frac{c_0}{n}}(G') \sum_{G:E(G')\subseteq E(G)} \mathbb{P}_{\frac{c_0}{n}\to\frac{c_1}{n}}(G'\to G)q^*(G) \qquad (6.39)\end{aligned}$$

Write $q^*(G) = q^*(G') + q^*(G) - q^*(G')$ and we can rearrange (6.39) to get

$$\begin{aligned}&\mathbb{E}\big[q^*(G_{n,c_1/n})\big] - \mathbb{E}\big[q^*(G_{n,c_0/n})\big] \\ &\quad = \sum_{G'} \mathbb{P}_{\frac{c_0}{n}}(G') \sum_{G':E(G')\subseteq E(G)} \mathbb{P}_{\frac{c_0}{n}\to\frac{c_1}{n}}(G'\to G)(q^*(G) - q^*(G')) \qquad (6.40)\end{aligned}$$

It only remains to show that the RHS of (6.40) is small in absolute value. There are two cases. Firstly if $e(G) - e(G') \geq 2\delta n$ then $\mathbb{P}_{\frac{c_0}{n}\to\frac{c_1}{n}}(G' \to G) < \varepsilon/2$. Secondly if $e(G) - e(G') < 2\delta n$ then by Lemma 1.4.5 $|q^*(G) - q^*(G')| < \varepsilon/2$. Hence the RHS of (6.40) has absolute value less than ε and we are done. $\square$

6.7 Literature on random graphs

The original paper is Erdős and Rényi [22] which initiated the study of random graphs. Already in this paper the likely sizes of the connected components were established for three ranges, see Lemma 6.1.2. The model of random graphs actually presented in [22] was the $\mathcal{G}(n,m)$ model where a random graph is chosen uniformly from all labelled graphs with m edges on n vertices. However, there is a connection between the random graphs $\mathcal{G}(n,p)$ and $\mathcal{G}(n,m)$ when $m = \binom{n}{2}p$ (see the text [31]) and so [22] is considered to have effectively begun the study of the $\mathcal{G}(n,p)$ model.

Let's recall the state of play after the 1960 paper [22]. For c a constant and $p = c/n$ the likely sizes of the largest connected component was known for $c < 1$, $c = 1$ and $c > 1$ to be $O(\log n)$, $\Theta(n^{2/3})$, and $\Theta(n)$ respectively. In papers by Bollobás [6] and Łuczak [42], the notion of a critical window about $p = 1/n$ was introduced, see Lemma 6.1.3. This further refined the probabilities considered and allowed study of the transition in the size of the largest connected component from $O(\log n)$ to order $n^{2/3}$ and from (possibly many) connected components with size of order $n^{2/3}$ to a single component of linear size. More precisely the appropriate scaling is to set $p = \frac{1}{n}(1 + \gamma)$ where $\gamma = o(1)$ and then the random graph exhibits different behaviours in the three regimes $\gamma^3 n \to -\infty$, $\gamma^3 n = O(1)$ and $\gamma^3 n \to \infty$. The first and last of these are called the lower and upper window respectively.

The study of random graphs has remained active. There are too many interesting results to do any justice to this area so from now on we take a mercenary approach and present only those which are directly applicable to our analysis of the modularity of random graphs.

The modularity of a graph can be determined from the partial modularity of its connected components (see Lemma 1.6.2). Hence it is important to know the likely number of edges and structure of these components in our random graph. We start with results on the structure of the components.

The excess of a connected component H is defined to be $\ell(H) = e(H) - |H|$. Whenever this excess is strictly positive, i.e. H not a tree or a unicyclic graph, we say H is a complex component. The likely complexities of the connected components are different for the three stages of the critical window. We begin with the lower window. The next three results were first developed in [6, 42, 43]. However we will quote the references from the book on random graphs by Janson, Łuczak and Ruciński [31].

Lemma 6.7.1 (Theorem 5.5 [31]). *Let $np = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to -\infty$ and suppose $G_n \sim \mathcal{G}(n, p)$. Then whp G_n has no complex components.*

The trees and unicyclic components in the lower window then give way to (possibly many) complex component(s), although these form a small portion of the graph and the overall excess of the graph is still small.

Lemma 6.7.2 (Theorem 5.19 [31]). *Let $np \leq 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n = O(1)$ and suppose $G_n \sim \mathcal{G}(n, p)$. Then whp the excess is $\ell(G_n) = O(1)$ and all complex components in G_n have $O(n^{2/3})$ vertices combined.*

The (possibly many) component(s) with positive excess in the central region of the critical window then likely give way to one single complex component in the upper window. We combine the results of three theorems from [31], see the note at the top of p119 of the same book.

Lemma 6.7.3 (Theorems 5.7, 5.8 and 5.10 [31]). *Let $np = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$ and suppose $G_n \sim \mathcal{G}(n, p)$. Then whp the G_n has exactly one complex component of size $\Omega(n^{2/3})$ with all other components of size $O(n^{2/3})$.*

Thus in the upper window whp the largest component is of a different structure and size to the other components in the graph. And recall for $p = c/n$ with $c > 1$ constant we have a unique component of linear size with other components of size $O(\log n)$. In these two ranges of p we need to analyse the largest connected component separately to the rest of the graph. We start with a result on the likely size of the largest component.

Lemma 6.7.4 (Bollóbas [6], Łuczak [42]). *Let $(np - 1)n^{1/3} \to \infty$ and $\limsup np < \infty$ and suppose $G_n \sim \mathcal{G}(n, p)$. Write $c = np$ and define $t \in (0, 1)$ by $te^{-t} = ce^{-c}$. Then whp the largest connected component H in G_n satisfies*

$$|H| = \left(1 - \frac{t}{c}\right) n(1 + o(1))$$

and the second largest component is of size $O(n^{2/3})$.

As well as the size of the giant component it is also useful to know the likely number of edges inside and the excess of the giant. Both Lemma 6.7.5 and Lemma 6.7.6 follow from Theorem 6 in Pittel and Wormald's paper [53].

Lemma 6.7.5 (Pittel and Wormald [53]). *Let $k \leq np \leq K$ for constants $k, K > 1$ and suppose $G_n \sim \mathcal{G}(n,p)$. Write $c = np$ and define $t \in (0,1)$ by $te^{-t} = ce^{-c}$. Then whp the largest connected component H in G_n satisfies*

$$e(H) = \frac{(1-t/c)(c+t)}{2}(1+o(1)),$$

and

$$\ell(H) = \frac{(1-t/c)(c+t-2)}{2}(1+o(1)).$$

We note the likely number of edges in the giant component is also given explicitly by Janson and Luczak in Theorem 2.3 and the discussion in Section 3 of their paper [30].

Detailed results for the joint distribution of the size, edge count, and excess of the giant component for the upper window of the critical phase are also contained in Theorem 6 of [53]. In the paper the result is stated in terms of different variables. Below, following 'note 4' of [53], we have made the subsitution $t = 1-\gamma+2\gamma^2/3+O(\gamma^3)$ which holds in the case of p in the upper window. The expectations and co-variance matrix agree with those in 'note 4' of the paper, but we give more terms of the expansion.

Lemma 6.7.6 (Pittel and Wormald [53]). *Let $np = 1+\gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$ and suppose $G_n \sim \mathcal{G}(n,p)$. Whp G_n has a unique giant component H and we let Y_1, Y_2, Y_3 be random variables counting the number of vertices in the 2-core of H, the number of vertices in the tree mantle of H and the excess of H respectively. Then*

$$\mathbb{E}(Y_1) = 2\gamma^2 n - 4\gamma^3 n + O(\gamma^4 n), \quad \mathbb{E}(Y_2) = 2\gamma n - \tfrac{14}{3}\gamma^2 n + O(\gamma^3 n), \quad \mathbb{E}(Y_3) = \tfrac{2}{3}\gamma^3 n + O(\gamma^4 n)$$

with co-variance matrix,

$$\begin{pmatrix} 12\gamma - 39\frac{1}{3}\gamma^2 + O(\gamma^3) & 4 - 23\frac{1}{3}\gamma + O(\gamma^2) & 6\gamma^2 - 18\frac{2}{3}\gamma^3 + O(\gamma^4) \\ 4 - 23\frac{1}{3}\gamma + O(\gamma^2) & \dfrac{2}{\gamma} - 12 + O(\gamma) & 2\gamma - 11\frac{1}{3}\gamma^2 + O(\gamma^3) \\ 6\gamma^2 - 18\frac{2}{3}\gamma^3 + O(\gamma^4) & 2\gamma - 11\frac{1}{3}\gamma^2 + O(\gamma^3) & \frac{10}{3}\gamma^3 n + O(\gamma^4 n) \end{pmatrix} n.$$

From Lemma 6.7.6 we need only the likely distribution of the edge count and excess of the giant component. We collate these in Corollaries 6.7.7 and 6.7.8 respectively.

Corollary 6.7.7. *Let $np = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$ and suppose $G_n \sim \mathcal{G}(n,p)$. Whp G_n has a unique giant component H. And whp for any $\omega \to \infty$,*

$$e(H) = 2\gamma n \left(1 - \frac{4\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right).$$

Observe that we can take $\omega = (\gamma^3 n)^{\frac{1}{10}}$ for example, and so the corollary implies that whp the number of edges in the young giant is $2\gamma n(1 + o(1))$.

Proof. If we let $\mu = \mathbb{E}(e(H))$ and $\sigma^2 = \mathrm{Var}(e(H))$ then by Chebyshev's inequality

$$\mathbb{P}\left(|e(H) - \mu| \geq k\sigma\right) \leq \frac{1}{k^2}.$$

Notice that in the notation of Lemma 6.7.6, $e(H) = Y_1 + Y_2 + Y_3$. Hence, by Lemma 6.7.6 we can take $\mu = 2\gamma n(1 - \frac{4\gamma}{3}) + O(\gamma^3 n)$ and $\sigma = O\left(\sqrt{\frac{n}{\gamma}}\right)$ and thus whp

$$\left|e(H) - 2\gamma n\left(1 - \frac{4\gamma}{3}\right)\right| \leq O(\gamma^3 n) + O\left(\omega\sqrt{\frac{n}{\gamma}}\right).$$

After rearranging we get that whp

$$e(H) = 2\gamma n \left(1 - \frac{4\gamma}{3} + O(\gamma^2) + O\left(\frac{\omega}{\sqrt{\gamma^3 n}}\right)\right).$$

□

The likely excess also follows from the expectation and variance given in Lemma 6.7.6.

Corollary 6.7.8. *Let $np = 1 + \gamma$ where $\gamma = o(1)$ and $\gamma^3 n \to \infty$ and suppose $G_n \sim \mathcal{G}(n,p)$. Let $\omega \to \infty$. Then whp G_n has a unique giant component H with excess*

$$\ell(H) = \frac{2\gamma^3 n}{3}\left(1 + O(\gamma) + O\left(\frac{\omega}{(\gamma^3 n)^{\frac{1}{2}}}\right)\right).$$

Proof. The proof follows by Chebyshev's inequality in the same manner as the proof of Corollary 6.7.7. By Chebyshev whp

$$|\ell(H) - \mathbb{E}(\ell(H))| \leq \omega\sqrt{\mathrm{Var}(\ell(H))}. \tag{6.41}$$

By the result of Pittel and Wormald, Lemma 6.7.6, we may take $\mathbb{E}(\ell(H)) = 2\gamma^3 n(1+O(\gamma))/3$ and $\mathrm{Var}(\ell(H)) = O(\gamma^3 n)$ and then the result follows by (6.41). □

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