Generating and counting Hamilton cycles in random regular graphs

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1 Introduction

This paper deals with computational problems involving Hamilton cycles in random regular graphs. Thus let $\mathcal{G} = \mathcal{G}(r,n)$ denote the set of r-regular (simple) graphs with vertex set $[n] = \{1, 2, ..., n\}$. While it is NP-Complete to tell whether or not a cubic (r = 3) graph has a Hamilton cycle, it has been known for some time that for r fixed but sufficiently large, G chosen at random from $\mathcal{G}(r,n)$ is Hamiltonian \mathbf{whp}^1 , see Bollobás [2], Fenner and

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¹An event \mathcal{E}_n is said to occur **whp** (with high probability) if $\mathbf{Pr}(\mathcal{E}_n) = 1 - o(1)$ as

Frieze [5]. These results were non-constructive and Frieze [6] described an $O(n^3 \log n)$ time algorithm that found a Hamilton cycle **whp**, provided $r \ge 85$. Thus until quite recently it was not known whether or not a random cubic graph was Hamiltonian **whp**. (Experiments with the algorithm of [6] strongly suggested that it was.)

In two recent papers Robinson and Wormald [12], [13] used a second moment approach and showed that random r-regular graphs are Hamiltonian **whp** for $r \geq 3$. Their proof is non-constructive and the purpose of this paper is to provide corresponding algorithmic results. We abandon the rotation-extension approach of [6] in favour of an approach based on rapidly mixing Markov chains. We prove

Theorem 1 Let $r \geq 3$ be fixed and let G be chosen uniformly at random from $\mathcal{G}(r,n)$. There is a polynomial time algorithm FIND which constructs a Hamilton cycle in G whp.

For a graph G let HAM(G) denote the set of Hamilton cycles of G. Assuming $HAM(G) \neq \emptyset$, a near uniform generator for HAM(G) is a randomised algorithm which on input $\epsilon > 0$ outputs a cycle $H \in HAM(G)$ such that for any fixed $H_1 \in HAM(G)$

$$\left| \mathbf{Pr}(H = H_1) - \frac{1}{|\mathrm{HAM}(G)|} \right| \le \frac{\epsilon}{|\mathrm{HAM}(G)|}.$$
 (1)

The probabilities here are with respect to the algorithm's random choices, as G is considered fixed in (1). The algorithm is polynomial if it runs in time polynomial in n and $1/\epsilon$.

Theorem 2 Let $r \geq 3$ be fixed. There is a procedure GENERATE such that if G is chosen uniformly at random from $\mathcal{G}(r,n)$ then **whp** GENERATE is a polynomial time generator for HAM(G).

Given a polynomial time generator for a set X one can usually estimate its size. This notion is made precise in Jerrum, Valiant and Vazirani [10]. The results there are based on the notion of self-reducibility (Schnorr [14]), which we do not have here. On the other hand, our method of proof does lead to an FPRAS (Fully Polynomial Randomised Approximation Scheme) for almost every $G \in \mathcal{G}(r,n)$.

An FPRAS for HAM(G) is a randomised algorithm which on input $\epsilon, \delta > 0$ produces an estimate Z such that

$$\mathbf{Pr}\left(\left|\frac{Z}{|\mathrm{HAM}(G)|} - 1\right| \ge \epsilon\right) \le \delta. \tag{2}$$

Again, the probabilities in (2) are with respect to the algorithm's choices. The running time of the algorithm is polynomial in $n, 1/\epsilon$ and $\log(1/\delta)$.

Theorem 3 Let $r \geq 3$ be fixed. There is a procedure COUNT such that if G is chosen uniformly at random from $\mathcal{G}(r,n)$ then **whp** COUNT is an FPRAS for HAM(G).

These results can be extended to random regular digraphs, see Frieze, Molloy and Cooper [7], Janson [8] for the non-constructive counterparts.

Our final result concerns a problem left open by Broder, Frieze and Shamir [4]. A graph G with vertex set [n] is obtained by adding a random perfect matching M to a random Hamilton cycle H. The problem is to find a Hamilton

cycle in G without knowing H. One motivation for this problem is in the design of authentication protocols. Our positive result on finding a Hamilton cycle can be viewed as a negative result for such a protocol.

Theorem 4 Let n be even and let G be obtained as the union of a random perfect matching M and a random (disjoint) Hamilton cycle H. Applying FIND to G will lead to the construction of a Hamilton cycle \mathbf{whp} .

The next section outlines the proof of these results and the remaining sections fill in the missing details.

2 Outline proofs of Theorems

2.1 Configurations

Initially we will not work directly with $\mathcal{G}(r,n)$. Instead we will use the configuration model as developed by Bender and Canfield [1] and Bollobás [3]. Thus let $W = [n] \times [r]$ ($W_v = v \times [r]$ represents r half edges incident with vertex $v \in [n]$.) The elements of W are called points and a 2-element subset of W is called a pairing. A configuration F is a partition of W into rn/2 pairings. We associate with F a multigraph $\mu(F) = ([n], E(F))$ where, as a multi-set,

$$E(F) = \{(v,w): \{(v,i),(w,j)\} \in F \text{ for some } 1 \leq i,j \leq r\}.$$

(Note that v = w is possible here.)

Let Ω denote the set of possible configurations. Thus

$$|\Omega|=P(rn)$$

where

$$P(2m) = \frac{(2m)!}{m!2^m}.$$

We say that F is simple if the multigraph $\mu(F)$ has no loops or multiple edges. Let Ω_0 denote the set of simple configurations.

We turn Ω into a probability space by giving each element the same probability. The main properties that we need of this model are

P1 Each $G \in \mathcal{G}(n,r)$ is the image (under μ) of exactly $(r!)^n$ simple configurations.

P2
$$Pr(F \in \Omega_0) \approx e^{-(r^2-1)/4}$$
.

(Here $\alpha \approx \beta$ means that $\alpha/\beta \to 1$ as $n \to \infty$.)

Suppose now that \mathcal{A}^* is a property of configurations and \mathcal{A} is a property of graphs such that when $F \in \Omega_0, \mu(F) \in \mathcal{A}$ implies $F \in \mathcal{A}^*$. Then P1 and P2 imply

$$\mathbf{Pr}(G \in \mathcal{A}) \le (1 + o(1))e^{(r^2 - 1)/4}\mathbf{Pr}(F \in \mathcal{A}^*)$$

where G is chosen randomly from \mathcal{G} and F is chosen randomly from Ω . We will generally use this to prove

$$\mathbf{Pr}(F \in \mathcal{A}^*) = o(1) \text{ implies } \mathbf{Pr}(G \in \mathcal{A}) = o(1).$$
 (3)

2.2 Generating and counting

We now begin the proof proper. For $F \in \Omega$ let

$$Z_H = Z_H(F) = |\mathrm{HAM}(\mu(F))|.$$

Then

$$\mathbf{E}(Z_H) = \frac{H(n,r)P((r-2)n)}{P(rn)},\tag{4}$$

where

$$H(n,r) = \frac{(n-1)!}{2} (r(r-1))^n.$$

Explanation: H(n,r) is the number of sets of n pairings which would be projected by μ to a Hamilton cycle (an H-configuration). P((r-2)n)/P(rn) is the probability that a given H-configuration appears in F.

Note that Stirling's approximation gives

$$\mathbf{E}(Z_H) pprox \sqrt{rac{\pi}{2n}} \left((r-1) \left(rac{r-2}{r}
ight)^{(r-2)/2}
ight)^n.$$

which grows exponentially with n for $r \geq 3$.

Using the method of Robinson and Wormald we prove (Section 5) that

$$Z_H \ge n^{-1} \mathbf{E}(Z_H) \quad \mathbf{whp}, \tag{5}$$

which by (3) implies

$$|\text{HAM}(G)| \ge \frac{1}{n} \mathbf{E}(Z_H) \text{ whp.}^2$$
 (6)

A 2-factor of a graph G is a set of vertex disjoint cycles which contain all vertices. Let 2FACTOR(G) denote the set of 2-factors of G. Then

$$HAM(G) \subseteq 2FACTOR(G)$$
.

²Robinson and Wormald prove this for r=3 but decline to do it for $r\geq 4$. They proceed indirectly. This has advantages and disadvantages. The advantage is that they show that a random r+1-regular graph is *close* to a random r-regular graph plus a random matching $(r\geq 2)$. But for our purposes, (6) is what is needed.

For $F \in \Omega$ let

$$Z_f = Z_f(F) = |2\text{FACTOR}(\mu(F))|.$$

Now

$$\mathbf{E}(Z_f) \le \frac{\binom{r}{2}^n P(2n)P((r-2)n)}{P(rn)}.$$
(7)

Explanation: there are $\binom{r}{2}^n$ ways of choosing two points from each W_v . There are then P(2n) ways of pairing these points. If the set X of n pairings contains no loops or multiple edges then μ projects X to a 2-factor. The remaining terms give the probability that X exists in F. We have inequality in (7) as some sets X do not yield 2-factors and some yield the same. On the other hand all 2-factors of G arise in this way. By the Markov inequality

$$Z_f \leq n\mathbf{E}(Z_f)$$
 whp,

which by (3) implies

$$|2\text{FACTOR}(G)| \le n\mathbf{E}(Z_f) \text{ whp.}$$
 (8)

Now by (4) and (7)

$$\frac{\mathbf{E}(Z_f)}{\mathbf{E}(Z_H)} \leq \frac{(2n)!}{2^{2n-1}n!(n-1)!} \\
\leq 2n^{1/2}. \tag{9}$$

Combining (6) and (8) we obtain

$$\frac{|\mathrm{HAM}(G)|}{|\mathrm{2FACTOR}(G)|} \ge \frac{1}{2n^{5/2}} \ \mathbf{whp}. \tag{10}$$

We will show in Section 3 that **whp** there is a polynomial time generator and an FPRAS for 2FACTOR(G). This and (10) easily verifies Theorems 1,2 and 3. Indeed we estimate |2FACTOR(G)| and the ratio |HAM(G)|/|2FACTOR(G)|.

The former is estimated by the assumed FPRAS and the latter by generating $O(n^{5/2}/\epsilon^2)$ 2-factors and computing the proportion that are Hamilton cycles (ϵ is the required relative accuracy).

2.3 Hidden Hamilton cycles

Let $X = \{(H, M) : H \text{ is a Hamilton cycle, } M \text{ is a perfect matching of } K_n \text{ and } H \cap M = \emptyset\}$. Consider X to be a probability space in which each element is equally likely. Let \mathbf{Pr}_1 refer to probabilities in this space and \mathbf{Pr}_0 , \mathbf{E}_0 refer to probability and expectation with respect to F chosen randomly from Ω_0 .

Let $A = \{F \in \Omega_0 : \text{GENERATE} \text{ is not a polynomial time generator for } HAM(\mu(F))\}$ and $\hat{A} = \{(H, M) \in X : \text{GENERATE} \text{ is not a polynomial time generator for } HAM(H \cup M)\}$ be the corresponding subset of X. Now for each $(H, M) \in X$ there are 6^n configurations F for which $\mu(F) = H \cup M$ and for each $F \in \Omega_0$ there are $Z_H(F)$ corresponding pairs (H, M) in X. Thus, where 1_A is the indicator function of the set A,

$$\begin{aligned} \mathbf{Pr}_{1}(\hat{A}) &= \sum_{(H,M)\in\hat{A}} \frac{1}{|X|} \\ &= \sum_{F\in A} \frac{Z_{H}(F)}{6^{n}|X|} \\ &= \frac{1}{\mathbf{E}_{0}(Z_{H})} \mathbf{E}_{0}(1_{A}Z_{H}) \qquad \text{since } 6^{n}|X| = |\Omega_{0}|\mathbf{E}_{0}(Z_{H}) \\ &\leq \frac{1}{\mathbf{E}_{0}(Z_{H})} \sqrt{\mathbf{E}_{0}(1_{A}^{2})\mathbf{E}_{0}(Z_{H}^{2})}. \end{aligned}$$

 $^{^3}$ This elegant use of the Cauchy-Schwarz inequality was pointed out to us by Svante Janson.

Robinson and Wormald proved [11] that

$$\mathbf{E}_0(Z_H^2)pprox rac{3}{e}\,\mathbf{E}_0(Z_H)^2.$$

Hence

$$\mathbf{Pr}_{1}(\hat{A}) \leq (1 + o(1))\sqrt{3/e}\,\mathbf{Pr}_{0}(A)$$

$$= o(1), \tag{11}$$

by Theorem 1.

3 Generating and counting 2-factors

For any graph G = (V, E), a construction of Tutte [15] gives a graph G' = (V', E') such that the perfect matchings in G' correspond in a natural fashion to the 2-factors of G. Specifically, (assuming G is r-regular) for each vertex $v \in V$ we have a complete bipartite graph $H_v \cong K_{r,r-2}$ with bipartition

$$U_v = \{u_{v,w} : \{v,w\} \in E\}, \quad W_v = \{w_{v,i} : 1 \le i \le r-2\}.$$

Now $V' = \bigcup_{v \in V} (U_v \cup W_v)$ and E' contains the edge set of H_v for each $v \in V$. Additionally, for each edge $\{v, w\} \in E$ we have a unique edge $\{u_{v,w}, u_{w,v}\} \in E'$. We will call these the G-edges of G' and the remainder the H-edges.

In any perfect matching in G' exactly two vertices in U_v will not be matched by H-edges. They must therefore be matched by two G-edges incident with H_v . Thus the n G-edges in the matching correspond to a 2-factor K in G. For each such choice of edges, the remaining (r-2)n H-edges can be chosen in $(r-2)!^n$ ways. Therefore each 2-factor in G corresponds to $(r-2)!^n$ perfect matchings in G'. In particular, by generating a near uniform perfect

matching G' we can generate a near uniform 2-factor of G. Similarly, by approximately counting perfect matchings in G', we can approximately count 2-factors in G.

The problem of generating near uniform perfect matchings in a graph Γ was studied by Jerrum and Sinclair [9]. They describe an algorithm which runs in time polynomial in $|V(\Gamma)|$, $1/\epsilon$ and $\rho = \rho(\Gamma)$, where ρ is the ratio of the number of near perfect to perfect matchings of Γ (a near perfect matching covers all but two vertices). In light of this we have only to show that **whp** $\rho(G')$ is bounded by a polynomial in n.

Let ν_p and ν_{np} denote the number of perfect and near perfect matchings in G', assuming G is chosen at random from $\mathcal{G}(r,n)$. Then, from (6), we have

$$u_p \geq \frac{(r-2)!^n}{n} \mathbf{E}(Z_H)$$
 whp.

To estimate ν_{np} we consider the G-edges of some near perfect matching M' of G. Let M denote the corresponding set of edges in G itself. It is straightforward to verify that the subgraph G(M) induced by M has

- (i) n-2 vertices of degree 2, and
- (ii) 2 vertices with degrees $d_1, d_2 \in \{0, 1, 2, 3, 4\}$ where $d_1 + d_2 = 2, 4$ or 6.

Let Z_{nf} denote the number of subgraphs of G satisfying (i) and (ii). Clearly

$$\nu_{np} \le (r-2)!^{n-2} (r!)^2 Z_{nf} \tag{12}$$

and a (crude) argument similar to that for (7) yields

$$\mathbf{E}(Z_{nf}) \le \frac{\binom{n}{2} (r^4)^2 \binom{r}{2}^{n-2} \sum_{k=-1}^{1} P(2(n+k)) P((r-2)n - 2k)}{P(rn)}.$$

Applying (12) and the Markov inequality we see that

$$u_{np} \le n(r-2)!^{n-2}(r!)^2 \mathbf{E}(Z_{nf}) \quad \mathbf{whp}$$

and so whp

$$\rho(G') \leq \frac{n^2 \binom{n}{2} (r-2)!^{n-2} r!^2 r^8 \binom{r}{2}^{n-2} \sum_{k=-1}^{1} P(2(n+k)) P((r-2)n-2k)}{(r-2)!^n \mathbf{E}(Z_H) P(rn)} \\
= O(n^{9/2}),$$

as required.

4 The Variance of Z_H

The method of Robinson and Wormald is an analysis of variance. We will partition the probability space Ω into groups according to the number of cycles of each size. We will then show that $\mathbf{Var}(Z_H)$ can be "explained" almost entirely by the variance between groups. Thus, within most groups Z_H is concentrated around its mean, which in most groups is "close" to $\mathbf{E}(Z_H)$. In this section we compute the variance of Z_H .

We will from now on assume that $r \geq 4$. The case r = 3 has been dealt with in [12]. The calculations there are done directly on $\mathcal{G}(3, n)$.

We will count the number of potential pairs of Hamilton cycles by counting the number of pairs (H, H') of H-configurations whose intersection is a set of a paths containing a total of k edges, and summing over all feasible a, k. If H, H' coincide, then we have k = n and we take a = 0. Thus:

$$\mathbf{E}(Z_H^2) = \mathbf{E}(Z_H) \sum_{k,a} N(k,a) P((r-4)n + 2k) / P((r-2)n), \tag{13}$$

where N(k, a) is the number of ways of selecting H' given H, k and a. Note that this quantity is independent of H.

Explanation: for each fixed H, k, a the number of possible H' is independent of H. Taking out the factor $\mathbf{E}(Z_H)N(k,a)$ leaves us with $\mathbf{Pr}(H'\mid H)$ which comprises the last two factors.

Claim 1: The number of ways of selecting k edges from H consisting of a paths is

$$\frac{an}{k(n-k)} \binom{k}{a} \binom{n-k}{a}.$$

provided we interpret an/k(n-k) as 1 when a=0 (equivalently k=0 or k=n).

Proof We will assume a>0 and k< n. Fix an orientation of H. Remove any edge of H and insist that it is not one of the k edges. We now have a path of length n-1 from which we must choose k edges forming a paths. There are $\binom{k-1}{a-1}$ ways to choose the lengths of the paths, and $\binom{n-k}{a}$ ways to pick their initial vertices. There were n ways to choose the edge that was removed, and each choice of paths had n-k eligible choices for this edge. Therefore, the number of ways of selecting the paths is $\frac{n}{n-k}\binom{k-1}{a-1}\binom{n-k}{a}=\frac{an}{k(n-k)}\binom{k}{a}\binom{n-k}{a}$.

Claim 2: Given our choice of the k edges of H, the number of ways to complete H' is:

$$\left(rac{2(r-2)}{r-3}
ight)^a H(n-k,r-2).$$

Proof Imagine that each of these a paths is contracted to a single vertex. The selection of a Hamilton cycle H' extending the chosen fragments of H can be divided into two steps: (i) select a Hamilton cycle on n-k vertices

which joins up all the (contracted) fragments, and then (ii) select a way of splicing in the (expanded) fragments to obtain a full n-edge H-configuration H'. The number of choices in (i) is simply H(n-k,r-2), where we must interpret H(0,r-2) as 1, while for (ii) it is $(2(r-2)/(r-3))^a$. (For each fragment we may choose a direction of traversal; then, on expanding each fragment from a point to a path, the number of ways of connecting H' to the endpoints of a fragment is increased from (r-2)(r-3) — as counted by the formula for H(n-k,r-2) — to $(r-2)^2$.)

Substituting for N(k, a) in (13), and applying (4) and Stirling's formula, we have

$$\mathbf{E}(Z_{H}^{2}) = \mathbf{E}(Z_{H}) \sum_{Q} \frac{an}{k(n-k)} \binom{k}{a} \binom{n-k}{a} \left(\frac{2(r-2)}{r-3}\right)^{a} \times \frac{H(n-k,r-2)P((r-4)n+2k)}{P((r-2)n)},$$

$$\approx \frac{\sqrt{\pi n}}{4} \left(\frac{n}{e}\right)^{-(r-2)n/2} \left(\frac{(r-1)(r-2)(r-3)}{2^{(r-4)/2}r^{(r-2)/2}}\right)^{n} \times \sum_{Q} \frac{a}{k(n-k)^{2}} T_{a,k}, \tag{14}$$

where

$$T_{a,k} = \frac{k!(n-k)!^2((r-4)n+2k)!(r-2)^{a-k}2^{a-k}}{a!^2(k-a)!(n-k-a)!((r-4)n/2+k)!(r-3)^{a+k}},$$

and

$$Q = \{(k,a) \mid a, k-a, n-k-a \geq 0\}.$$

It is straightforward to check that we can ignore all terms on the border of Q, as they each contribute $o(n^{-2}\mathbf{E}(Z_H)^2)$, and so we define

$$Q' = \{(k, a) \mid a, k - a, n - k - a > 0\}.$$

Now set $\kappa = \frac{k}{n}$, $\alpha = \frac{a}{n}$. Using Stirling's approximation, we have:

$$\mathbf{E}(Z_H^2) \approx \frac{1}{4n^2} \left(\frac{2^{(r-4)/2}(r-1)(r-2)(r-3)}{r^{(r-2)/2}} \right)^n \times \sum_{Q'} F^n \lambda(1+\epsilon), \tag{15}$$

where $F = F_r(\kappa, \alpha)$ is defined by

$$F = \frac{2^{\kappa + \alpha} (r-2)^{\alpha - \kappa} g(\kappa) g(1-\kappa)^2 g(\frac{r}{2} - 2 + \kappa)}{(r-3)^{\kappa + \alpha} g(\alpha)^2 g(\kappa - \alpha) g(1-\kappa - \alpha)},$$

with $g(x) = x^x$,

$$\lambda = (\kappa(\kappa - \alpha)(1 - \kappa - \alpha)(1 - \kappa)^2)^{-\frac{1}{2}},$$

and

$$\epsilon = O\left(\frac{1}{a} + \frac{1}{k-a} + \frac{1}{n-k-a}\right).$$

We extend the domain of F_r to

$$R = \{(\alpha, \kappa) \mid \alpha, \kappa - \alpha, 1 - \kappa - \alpha > 0\},\$$

by defining g(0) = 1. It is straightforward to verify that F_r is continuous over R. We now wish to find its maximum, so we will look for the critical points of F_r in the interior of R. We set the partial derivatives of $\ln F_r$ with respect to κ and α equal to 0, yielding the two equations:

$$\kappa(1 - \kappa - \alpha)(r - 4 + 2\kappa) - (r - 2)(r - 3)(1 - \kappa)^{2}(\kappa - \alpha) = 0, \tag{16}$$

and

$$(r-3)\alpha^{2} - 2(r-2)(\kappa - \alpha)(1 - \kappa - \alpha) = 0.$$
 (17)

It is easily verified that $\kappa = \kappa_0 = 2/r$, $\alpha = \alpha_0 = 2(r-2)/r(r-1)$ is a solution of the simultaneous equations (16) and (17). As we now show, this solution is the only one in the interior of R.

Solving equation (16) for α , noting that the equation is linear in α , we obtain

$$\alpha = \frac{\kappa(\kappa - 1)[(r^2 - 5r + 8)\kappa - (r^2 - 6r + 10)]}{Q_r(\kappa)},$$
(18)

where

$$Q_r(\kappa) = (r^2 - 5r + 4)\kappa^2 - (2r^2 - 9r + 8)\kappa + (r^2 - 5r + 6).$$

Substituting this expression for α in equation (17) yields an equation of the form $P_r(\kappa)/Q_r(\kappa)^2 = 0$, where

$$P_r(\kappa) = (r-3)\kappa(\kappa-1)^2(r\kappa-2)P'_r(\kappa),$$

and

$$P'_r(\kappa) = (r^3 - 10r^2 + 25r - 16)\kappa^2 + (-2r^3 + 16r^2 - 36r + 22)\kappa + (r^3 - 8r^2 + 20r - 16).$$
(19)

Clearly, any solution to (16) and (17) will also be a solution to $P_r(\kappa) = 0$.

When $\kappa = \kappa_0 = 2/r$, the solution $\alpha = \alpha_0$ is unique, except in the case r = 4, when equation (16) holds for all α and equation (17) allows the additional solution $\alpha = 1$ which is not in the interior of R. Clearly the roots $\kappa = 0$ and $\kappa = 1$ do not lead to solutions in the interior of R.

We have considered all roots of $P_r(\kappa)$, except those given by the quadratic (19). Our aim is to show that all such roots κ lead to solution pairs (α, κ) that do not lie in the interior of R. In analysing the quadratic $P'_r(\kappa)$, it is convenient

to assume $r \geq 7$, and leave r = 4, 5, 6 as special cases to be treated later. We first establish a lower bound on roots κ of equation (19), by recasting (19) in the form

$$P'_r(\kappa) = (r^3 - 10r^2 + 25r - 16)(\kappa - 1)^2 - (4r^2 - 14r + 10)\kappa + (2r^2 - 5r).$$

Under the assumption $r \geq 7$, the factor $r^3 - 10r^2 + 25r - 16$ is strictly positive, and hence any root κ of $P'_r(\kappa) = 0$ must satisfy

$$\kappa \geq \frac{2r^2 - 5r}{4r^2 - 14r + 10} > \frac{1}{2}.$$

Now, from equation (18),

$$1 - \kappa - \alpha = \frac{-(r-2)(r-3)(2\kappa - 1)(\kappa - 1)^2}{Q_r(\kappa)}.$$
 (20)

In the light of our lower bound on κ , we see immediately that the numerator of (20) is negative. We show that, for $r \geq 7$, the denominator of (20) is positive, from which it follows that $1 - \kappa - \alpha$ is negative, and the point (α, κ) cannot lie in the interior of R.

By direct calculation,

$$(2r-5)Q_r(\kappa) - 2P'_r(\kappa)$$

$$= (5r^2 - 17r + 12)\kappa^2 - (4r^2 - 11r + 4)\kappa + (r^2 - 3r + 2).$$
 (21)

The discriminant of quadratic (21) is $-(2r-5)(r-4)(2r^2-7r+4)$, which is negative for all r>4; furthermore, the leading coefficient of (21) is positive under the same condition on r. It follows that $(2r-5)Q_r(\kappa)-2P'_r(\kappa)$ is positive for all r>4 and all κ , and hence that $Q_r(\kappa)$ is positive for all r>4

and all κ satisfying $P'_r(\kappa) = 0$. This verifies the claim that the denominator of (20) is positive, and completes the analysis of the case $r \geq 7$.

The case r=5 may be eliminated by noting that, of the two roots $\kappa=(-1\pm\sqrt{10}\,)/4$ of (19), one is negative, and the other yields a corresponding value for α that is greater than 1. A similar argument eliminates the case r=6. When r=4, the two roots of (19) are $\kappa=0$ and $\kappa=1/2$; the former leads to a solution not in the interior R, while the latter is just a repeat of the root $\kappa=\kappa_0=2/r$ that we have already considered.

Now that we have established (κ_0, α_0) as the only critical point of F_r in R, other than (0,0), we will see that it is a local maximum, and it will follow that we can ignore all (κ, α) not nearby (κ_0, α_0) . Set

$$\delta_k = rac{k - \kappa_0 n}{\sqrt{n}}, \delta_a = rac{a - lpha_0 n}{\sqrt{n}},$$

and perform a Taylor expansion of $\ln(F_r(\kappa, \alpha))$ around (κ_0, α_0) , yielding:

$$F^n = F_r(\kappa_0, \alpha_0)^n \exp(-(A\delta_k^2 + B\delta_k\delta_a + C\delta_a^2) + \text{cubic terms and greater}),$$

where

$$A = \frac{1}{2(\kappa_0 - \alpha_0)} + \frac{1}{2(1 - \kappa_0 - \alpha_0)} - \frac{1}{2\kappa_0} - \frac{1}{1 - \kappa_0} - \frac{1}{r - 4 + 2\kappa_0},$$

$$B = \frac{1}{1 - \kappa_0 - \alpha_0} - \frac{1}{\kappa_0 - \alpha_0},$$

$$C = \frac{1}{\alpha_0} + \frac{1}{2(\kappa_0 - \alpha_0)} + \frac{1}{2(1 - \kappa_0 - \alpha_0)}.$$

Substituting $\kappa_0 = 2/r, \alpha_0 = 2(r-2)/r(r-1)$ we get:

$$A = \frac{r(r^4 - 9r^3 + 28r^2 - 34r + 16)}{4(r-2)^2(r-3)},$$

$$B = -rac{r(r-1)^2(r-4)}{2(r-2)(r-3)},$$
 $C = rac{r(r-1)^2}{4(r-3)}.$

The determinant $D=4AC-B^2$ of the Hessian of $A\delta_k^2+B\delta_k\delta_a+C\delta_a^2$ is

$$D = \frac{r^3(r-1)^2}{4(r-2)(r-3)}.$$

Now it is easily checked that A > 0 for $r \ge 4$ and since D > 0 we have that F is strictly concave, and (κ_0, α_0) is a local maximum. It follows that we can ignore all terms of (15) outside of

$$X = \{(k, a) \mid |k - \kappa_0 n|, |a - \alpha_0 n| \le \sqrt{n} \log n\}.$$

Now,

$$F_r(\kappa_0, lpha_0) = rac{(r-1)(r-2)^{r-3}}{2^{(r-4)/2}(r-3)r^{(r-2)/2}},$$

and so by (15),

$$\begin{split} \mathbf{E}(Z_H^2) &\approx \frac{1}{4n^2} \left(\frac{2^{(r-4)/2}(r-1)(r-2)(r-3)}{r^{(r-2)/2}} \right)^n \sum_X F(\kappa,\alpha)^n \lambda \\ &\approx \frac{1}{4n^2} \left(\frac{2^{(r-4)/2}(r-1)(r-2)(r-3)}{r^{(r-2)/2}} \right)^n \\ &\qquad \times \left(\frac{r^{5/2}(r-1)}{2(r-2)^{3/2}(r-3)^{1/2}} \right) F(\kappa_0,\alpha_0)^n \\ &\qquad \times n \int_X \exp\{-(A\delta_k^2 + B\delta_k\delta_a + C\delta_a^2)\} \, d\delta_k \, d\delta_a \\ &\approx \frac{1}{4n} \left(\frac{r^{5/2}(r-1)}{2(r-2)^{3/2}(r-3)^{1/2}} \right) \end{split}$$

$$\times \left(\left(\frac{r-2}{r} \right)^{r-2} (r-1)^2 \right)^n \frac{2\pi}{\sqrt{D}}$$

$$= \frac{\pi r}{2(r-2)n} \left(\left(\frac{r-2}{r} \right)^{r-2} (r-1)^2 \right)^n,$$

and comparing with (4), we have

$$\frac{\mathbf{E}(Z_H^2)}{\mathbf{E}(Z_H)^2} \approx \frac{r}{r-2}.$$
 (22)

5 Bounding Z_H whp

In the following, b, x are considered to be arbitrary large fixed positive integers. Let C_l denote the number of ℓ -cycles of $\mu(F)$ for $\ell \geq 1$. We will be concerned mainly with C_l where l is odd. For $\mathbf{c} = (c_1, c_2, \ldots, c_b) \in N^b$, where $N = \{0, 1, 2, \ldots\}$, let group $\Omega_{\mathbf{c}} = \{F \in \Omega : C_{2k-1} = c_k, 1 \leq k \leq b\}$. Let

$$\lambda_k = rac{(r-1)^{2k-1}}{2(2k-1)}.$$

It is straightforward to show that the $C_{\ell}, \ell \geq 1$, are asymptotically independent Poisson variables with mean $(r-1)^{\ell}/2\ell$; thus if **c** is fixed, then

$$\pi_{f c} = {f Pr}(F \in \Omega_{f c}) pprox \prod_{k=1}^b rac{\lambda_k^{c_k} e^{-\lambda_k}}{c_k!}.$$

Now let

$$S(x) = \{ \mathbf{c} \in N^b : c_k \le \lambda_k + x \lambda_k^{2/3}, 1 \le k \le b \},$$

and

$$\overline{\Omega} = igcup_{\mathbf{c}
ot\in S(x)} \Omega_{\mathbf{c}}.$$

Let

$$\overline{\pi} = \mathbf{Pr}(F \in \overline{\Omega}).$$

For $\mathbf{c} \in N^b$ let

$$E_{\mathbf{c}} = \mathbf{E}(Z_H \mid F \in \Omega_{\mathbf{c}})$$

and

$$V_{\mathbf{c}} = \mathbf{Var}(Z_H \mid F \in \Omega_{\mathbf{c}}).$$

Then we have

$$\mathbf{E}(Z_H^2) = \sum_{\mathbf{c} \in N^b} \pi_{\mathbf{c}} V_{\mathbf{c}} + \sum_{\mathbf{c} \in N^b} \pi_{\mathbf{c}} E_{\mathbf{c}}^2.$$
 (23)

The following two lemmas contain the most important observations. Lemma 1 shows that for most groups, the group mean is large and Lemma 2 shows that most of the variance can be explained by the *variance between groups*.

Lemma 1 For all sufficiently large x

- (a) $\overline{\pi} \leq e^{-\alpha x}$ for some absolute constant $\alpha > 0$.
- (b) $\mathbf{c} \in S(x)$ implies $E_{\mathbf{c}} \geq e^{-(\beta+\gamma x)} \mathbf{E}(Z_H)$, for some absolute constants $\beta, \gamma > 0$.

Lemma 2 If x is sufficiently large then

$$\sum_{\mathbf{c} \in S(x)} \pi_{\mathbf{c}} E_{\mathbf{c}}^2 \ge \left(1 - be^{-3\gamma x}\right) \left(1 - \left(\frac{2}{r-1}\right)^{2b}\right) \left(\frac{r}{r-2}\right) \mathbf{E}(Z_H)^2.$$

where γ is as in Lemma 1

Hence we have from (22) and (23) and Lemma 2,

$$\sum_{\mathbf{c} \in N^b} \pi_{\mathbf{c}} V_{\mathbf{c}} \le \delta \, \mathbf{E}(Z_H)^2, \tag{24}$$

where $\delta = \left(be^{-3\gamma x} + (\frac{2}{r-1})^{2b}\right) \frac{r}{r-2}$. The rest is an application of the Chebycheff inequality. Define the random variable \hat{Z}_H by

$$\hat{Z}_H = E_{\mathbf{c}}, \text{ if } F \in \Omega_{\mathbf{c}}.$$

Then for any t > 0

$$\begin{aligned} \mathbf{Pr}(|Z_H - \hat{Z}_H| \geq t) &\leq \mathbf{E}((Z_H - \hat{Z}_H)^2/t^2) \\ &= \sum_{\mathbf{c} \in N^b} \pi_{\mathbf{c}} V_{\mathbf{c}}/t^2 \\ &\leq \delta \mathbf{E}(Z_H)^2/t^2 \end{aligned}$$

where the last inequality follows from (24).

Put $t = e^{-(\beta + \gamma x)} \mathbf{E}(Z_H)/2$ where β, γ are from Lemma 1. Applying Lemma 1 we obtain that for n large,

$$\mathbf{Pr}\left(Z_{H} \geq \frac{\mathbf{E}(Z_{H})}{n}\right) \geq \mathbf{Pr}(Z_{H} \geq e^{-(\beta+\gamma x)}\mathbf{E}(Z_{H})/2)$$

$$\geq \mathbf{Pr}(|Z_{H} - \hat{Z}_{H}| \leq t \wedge (F \notin \overline{\Omega}))$$

$$\geq 1 - 4\delta e^{2(\beta+\gamma x)} - \overline{\pi}$$

$$\geq 1 - 4\delta e^{2(\beta+\gamma x)} - e^{-\alpha x}.$$

Hence,

$$\lim_{n\to\infty} \mathbf{Pr}\left(Z_H \ge \frac{\mathbf{E}(Z_H)}{n}\right) \ge 1 - \left(4be^{2\beta - \gamma x} + 4\left(\frac{2}{r-1}\right)^{2b}e^{2(\beta + \gamma x)}\right) \frac{r}{r-2} - e^{-\alpha x}.$$
(25)

This is true for all b, x and so the left hand side limit of (25) must in fact be one, proving (5), (putting $b = x^2$ and x arbitrarily large makes the right-hand side of (25) arbitrarily close to 1).

All that remains are the proofs of Lemmas 1 and 2

Proof of Lemma 2:

Let H_0 be some fixed Hamilton cycle.

$$E_{\mathbf{c}} = \sum_{F \in \Omega_{\mathbf{c}}} \frac{1}{|\Omega_{\mathbf{c}}|} \sum_{H \subseteq F} 1$$

$$= \sum_{H} \sum_{F \supseteq H \atop F \in \Omega_{\mathbf{c}}} \frac{1}{|\Omega_{\mathbf{c}}|} \frac{|\Omega|}{|\Omega|}$$

$$= \frac{|\Omega|}{|\Omega_{\mathbf{c}}|} \sum_{H} \mathbf{Pr}(F \supseteq H \text{ and } F \in \Omega_{\mathbf{c}})$$

$$= \frac{\mathbf{Pr}(F \supseteq H_{0})}{\mathbf{Pr}(\Omega_{\mathbf{c}})} \sum_{H} \mathbf{Pr}(F \in \Omega_{\mathbf{c}} \mid F \supseteq H)$$

$$= \frac{\mathbf{E}(Z_{H})\mathbf{Pr}(F \in \Omega_{\mathbf{c}} \mid F \supseteq H_{0})}{\mathbf{Pr}(\Omega_{\mathbf{c}})}.$$
(26)

So we will now compute $\mathbf{Pr}(F \in \Omega_{\mathbf{c}} \mid F \supseteq H_0)$, by first computing the expected number of cycles of length l, conditional on F containing H_0 . Here l can be considered fixed as $n \to \infty$.

To choose a cycle C of length l, we will first fix s, the number of edges in $C \cap H_0$ (hereafter called H-edges), and t, the number of H-paths, i.e. the paths formed by the H-edges.

First we will count the number of ways to choose the edges of C which will form the H-paths. Fix a starting vertex of C, and an orientation. We will

insist that the last edge of this orientation does *not* lie in an H-path. This will have the effect of multiplying the number of choices by 2(l-s). Now we will consider the generating function in which x, y, z mark the number of edges, H-edges, and H-paths respectively.

We go around the cycle and at each point we decide whether the next edge lies outside of H_0 , an option we represent by x, or if it is the first edge of an H-path, an option which we represent by $x^{i+1}y^iz$ where i is the length of the H-path. Note that the first edge following the H-path must of course lie outside of H_0 , explaining the exponent of x. Thus we find that the number of choices of H-edges in C is (where as usual $[x^ly^sz^t]$ stands for "coefficient of $x^ly^sz^t$ "):

$$egin{align} & [x^l y^s z^t] rac{1}{2(l-s)} \left(x + \sum_{i \geq 1} x^{i+1} y^i z
ight)^{l-s} \ & = & [x^l y^s z^t] rac{1}{2(l-s)} \left(x + rac{x^2 y z}{1-xy}
ight)^{l-s}. \end{split}$$

Given such a choice, we now compute the number of ways to finish the cycle. The number of ways to choose the sequence of vertices in the cycle is $\approx n^{l-s}2^t$. The number of choices for copies of those vertices is $(r-2)^{l-s+t}(r-3)^{l-s-t}$. Also, the number of configurations containing $H_0 \cup C$ is P((r-2)n-2(l-s)), so we multiply by:

$$pprox n^{l-s} 2^t (r-2)^{l-s+t} (r-3)^{l-s-t}$$
 $\times P((r-2)n - 2(l-s)) / P((r-2)n)$

$$pprox \quad \left(rac{2(r-2)}{r-3}
ight)^t (r-3)^{-s}(r-3)^l,$$

to get

$$[x^{l}y^{s}z^{t}] \frac{1}{2(l-s)} \left((r-3)x + \frac{2(r-2)x^{2}yz}{1-xy} \right)^{l-s}$$

$$= -\frac{1}{2} [x^{l}y^{s}z^{t}] \ln \left(1 - (r-3)x - \frac{2(r-2)x^{2}yz}{1-xy} \right).$$

(Observe that $((r-3)x+2(r-2)x^2yz/(1-xy))^k$ only contributes to terms of the form $x^i(x^2yz)^{k-i}(xy)^j$ for some i,j. So only i,j,k such that l=2k-i+j, s=k-i+j and t=k-i affect our expression. But this implies that k=l-s.)

Summing over all s, t (or equivalently putting y = z = 1), we get:

$$\begin{aligned} &-\frac{1}{2}[x^{l}]\ln\left(1-(r-3)x-\frac{2(r-2)x^{2}}{1-x}\right)\\ &=&-\frac{1}{2}[x^{l}]\ln\left(\frac{1-(r-2)x-(r-1)x^{2}}{1-x}\right)\\ &=&-\frac{1}{2}[x^{l}](\ln(1+x)+\ln(1-(r-1)x)-\ln(1-x))\\ &=&\frac{(r-1)^{l}+(-1)^{l}-1}{2l}.\end{aligned}$$

Note that for l even, this is equal to the unconditional expected number of l-cycles in F, explaining why we are concentrating on l odd. Let

$$\mu_k = rac{(r-1)^{2k-1} + (-1)^{2k-1} - 1}{2(2k-1)} = \lambda_k - rac{1}{2k-1},$$

the expected number of cycles of length 2k-1 in F conditional on $F\supseteq H_0$.

The next step is to compute

$$\mathbf{E}\left([C_3]_{i_3}[C_5]_{i_5}\dots[C_{2k-1}]_{i_{2k-1}}\mid F\supseteq H_0\right)$$

for any fixed $i_3, i_5, \ldots, i_{2k-1}$. This is done by counting the expected number of sets of i_3 distinct 3-cycles, i_5 distinct 5-cycles, ..., and i_{2k-1} distinct (2k-1)-cycles in F, conditional on $F \supseteq H_0$. It follows from a straightforward first moment argument that F a.s. has no two intersecting cycles of length at most k. It follows that the cycles appear almost independently, and we get:

$$\mathbf{E}\left([C_3]_{i_3}[C_5]_{i_5}\dots[C_{2k-1}]_{i_{2k-1}}\mid F\supseteq H_0\right)\approx\prod_{j=1}^k\mu_j^{i_j}.$$
 (27)

Therefore, conditional on $F \supseteq H_0$, the C_k are asymptotically independent Poisson variables with means μ_k . Hence, from (26),

$$E_{\mathbf{c}} \approx \mathbf{E}(Z_H) \prod_{k=1}^{b} \left(\frac{\mu_k}{\lambda_k}\right)^{c_k} e^{\lambda_k - \mu_k}.$$
 (28)

So,

$$\sum_{\mathbf{c} \in S(x)} \pi_{\mathbf{c}} E_{\mathbf{c}}^{2} \approx \mathbf{E}(Z_{H})^{2} \sum_{\mathbf{c} \in S(x)} \prod_{k=1}^{b} \left(\frac{\mu_{k}^{2}}{\lambda_{k}}\right)^{c_{k}} \frac{e^{-(2\mu_{k} - \lambda_{k})}}{c_{k}!}$$

$$= \mathbf{E}(Z_{H})^{2} \prod_{k=1}^{b} \sum_{c_{k}=0}^{\lambda_{k} + x\lambda_{k}^{2/3}} \left(\frac{\mu_{k}^{2}}{\lambda_{k}}\right)^{c_{k}} \frac{e^{-(2\mu_{k} - \lambda_{k})}}{c_{k}!}$$

$$= \mathbf{E}(Z_{H})^{2} \prod_{k=1}^{b} (1 - Z_{k}) e^{\frac{(\mu_{k} - \lambda_{k})^{2}}{\lambda_{k}}}$$

where

$$Z_{k} = \sum_{c_{k} = \lambda_{k} + x \lambda_{k}^{2/3}}^{\infty} \left(\frac{\mu_{k}^{2}}{\lambda_{k}}\right)^{c_{k}} \frac{e^{-(\mu_{k}^{2}/\lambda_{k})}}{c_{k}!}$$
(29)

The following lemma appears in [13]

Lemma 3 Let η_1, η_2, \ldots be given. Suppose that $\eta_1 > 0$ and that for some $c > 1, \eta_{i+1}/\eta_i > c$ for all i > 1. Then uniformly over $x \ge 1$,

$$R(x) = \sum_{i=1}^{\infty} \sum_{t=\eta_i(1+y_i)}^{\infty} \frac{\eta_i^t}{t! e^{\eta_i}} = O(e^{-c_0 x})$$

where $y_i = x\eta_i^{-1/3}$ and $c_0 = \min\{\eta_1^{1/3}, \eta_1^{2/3}\}/4$.

Applying this lemma with $\eta_i=\mu_i^2/\lambda_i$ and observing that $\eta_1=(r-3)^2/(2(r-1))\geq 6$ we see that

$$\sum_{k\geq 3} Z_k \leq \mathcal{O}(e^{-x/20})$$

Hence, for x sufficiently large,

$$\sum_{\mathbf{c} \in S(x)} \pi_{\mathbf{c}} E_{\mathbf{c}}^{2} \ge \mathbf{E}(Z_{H})^{2} (1 - be^{-x/20}) \prod_{k=1}^{b} \exp\left\{ \frac{(\mu_{k} - \lambda_{k})^{2}}{\lambda_{k}} \right\}.$$
(30)

Now,

$$\prod_{k=b+1}^{\infty} \exp\left\{\frac{(\mu_k - \lambda_k)^2}{\lambda_k}\right\} = \exp\left\{\sum_{k=b+1}^{\infty} \frac{2}{(2k-1)(r-1)^{2k-1}}\right\}$$

$$\leq \exp\left\{\frac{2}{(r-1)^{2b}}\right\}$$

$$\leq \left(1 - \frac{2}{(r-1)^{2b}}\right)^{-1}.$$

Thus, from (30), with

$$1- heta = \left(1-be^{-x/20}
ight)\left(1-rac{2}{(r-1)^{2b}}
ight),$$

$$\sum_{\mathbf{c} \in S(x)} \pi_{\mathbf{c}} E_{\mathbf{c}}^{2} \geq (1 - \theta) \mathbf{E}(Z_{H})^{2} \prod_{k=1}^{\infty} \exp\left\{\frac{(\mu_{k} - \lambda_{k})^{2}}{\lambda_{k}}\right\}$$

$$= (1 - \theta) \mathbf{E}(Z_{H})^{2} \exp\left\{\sum_{k=1}^{\infty} \frac{2}{(2k - 1)(r - 1)^{2k - 1}}\right\}$$

$$= (1 - \theta) \mathbf{E}(Z_{H})^{2} \left(\frac{r}{r - 2}\right).$$

Proof of Lemma 1

(a) Putting $\eta_i = \lambda_i$ satisfies the conditions of Lemma 3 with c = 4/3. Now

$$\overline{\pi} \leq \sum_{k=3}^{b} \sum_{c \geq \lambda_k (1+y_k)} \mathbf{Pr}(C_k = c)$$

$$\approx \sum_{k=1}^{b} \sum_{c \geq \lambda_k (1+y_k)} \frac{\lambda_k^c e^{-\lambda_k}}{c!}$$

$$= O(e^{-\alpha x}),$$

for some constant α , independent of x.

(b) Applying (28) we obtain

$$egin{array}{ll} E_{f c} &pprox & {f E}(Z_H) \prod_{k=1}^b \left(1-rac{2}{(r-1)^{2k-1}}
ight)^{c_k} \exp\left\{rac{1}{2k-1}
ight\} \ &\geq & AB^x, \end{array}$$

where

$$A = \prod_{k=1}^{b} \left(1 - rac{2}{(r-1)^{2k-1}}
ight)^{\lambda_k} \exp\left\{rac{1}{2k-1}
ight\}$$

and

$$B = \prod_{k=1}^{b} \left(1 - rac{2}{(r-1)^{2k-1}}
ight)^{\lambda_k^{2/3}}.$$

Now

$$A = \prod_{k=1}^{b} \exp\left\{\frac{1}{2k-1} - \left(\frac{2\lambda_k}{(r-1)^{2k-1}} + \frac{4\lambda_k}{2(r-1)^{2(2k-1)}} + \cdots\right)\right\}$$

$$\geq \prod_{k=1}^{\infty} \exp\left\{-\frac{2\lambda_k}{(r-1)^{2(2k-1)}}\right\}$$

$$= \exp\left\{-\sum_{k=1}^{\infty} \frac{1}{(2k-1)(r-1)^{2k-1}}\right\}.$$

The sum in the exponential term is convergent and so A is bounded below by a positive absolute constant.

Also

$$B \geq \prod_{k=1}^{\infty} \left(1 - \frac{2}{(r-1)^{2k-1}}\right)^{\lambda_k^{2/3}}$$
$$\geq \exp\left\{-\sum_{k=1}^{\infty} \frac{2}{(2k-1)^{\frac{2}{3}}(r-1)^{\frac{2k-1}{3}}}\right\}.$$

Again, the sum in the exponential term is convergent and so B is bounded below by a positive absolute constant, completing the proof.

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