On the chromatic number of a random 5-regular graph*†

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Abstract

It was only recently shown by Shi and Wormald, using the differential equation method to analyse an appropriate algorithm, that a random 5-regular graph asymptotically almost surely has chromatic number at most 4. Here, we show that the chromatic number of a random 5-regular graph is asymptotically almost surely equal to 3, provided a certain four-variable function has a unique maximum at a given point in a bounded domain. We also describe extensive numerical evidence which strongly suggests that the latter condition holds. The proof applies the small subgraph conditioning method to the number of locally rainbow balanced 3-colourings, where a colouring is *balanced* if the number of vertices of each colour is equal, and *locally rainbow* if every vertex is adjacent to at least one vertex of each of the other colours.

1 Introduction

The chromatic number of random regular graphs has attracted much interest in recent years. For the uniform model $\mathcal{G}_{n,d}$ of d-regular graphs on n labelled vertices, recent work has focussed on the chromatic number for fixed d. All necessary background with respect to random regular graphs as well as the pioneering results about their chromatic number and other parameters can be found in the comprehensive review paper by the last author [17].

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It is widely known that for $d \geq 2$ a random d-regular graph is a.a.s. not bipartite, and thus has chromatic number at least 3. (We say an event holds *asymptotically almost surely* (a.a.s.) if it holds with probability tending to 1 as $n \to \infty$. In these asymptotics for $\mathcal{G}_{n,d}$ we assume nd is always even for feasibility.) Molloy and Reed (see [10]) gave a lower bound on the chromatic number for general d, and in particular they showed that for a random 6-regular graph it is a.a.s. at least 4. The basic ingredient of the proof was the first moment method: showing that the expected number of 3-colourings of a random regular graph converges to zero.

Achlioptas and Moore [2] proved that random 4-regular graphs have chromatic number 3 w.p.p. (i.e. with probability bounded away from 0 for large n, which they refer to as 'with positive probability'). The proof was algorithmic in the sense that it used a backtracking-free algorithm based on Brelaz' heuristic. Subsequently, Achlioptas and Moore [3] showed that the chromatic number of a d-regular graph ($d \geq 3$) is a.a.s. k or $k+1$ or $k+2$, where k is the smallest integer such that $d < 2k \ln k$. They also showed that if furthermore $d > (2k-1)\ln k$, then a.a.s. the chromatic number is either $k+1$ or $k+2$. They also obtained an upper bound on the probability that it is $k+2$, which showed that 5-regular graphs can be 4-coloured w.p.p. in the multigraph model that is commonly used to analyse random regular graphs. This was subsequently improved by Shi and the last author [14, 15], who showed that the chromatic number of a random d-regular graph is a.a.s. 3 for $d = 4$, 4 for $d = 6$, and either 3 or 4 for $d = 5$. (In addition, they showed that a.a.s. the chromatic number of a d-regular graph, for all other d up to 10, is restricted to a range of two integers.) Their proofs were algorithmic.

The above results leave the main outstanding open question on the chromatic number of low-degree random regular graphs as follows: is the chromatic number of a 5-regular graph a.a.s. 3?

Previous attempts of some of the authors of the present paper to answer the above question in the negative, using refinements of the first moment method, failed. These attempts computed the expected number of successively more restricted types of 3-colourings (such that whenever a generic 3-colouring exists, at least one of the restricted type exists as well), and aimed at proving that it is a.a.s. equal to zero. All attempts however gave expected values that tend to ∞.

These failures also led to various innovative attempts to design an algorithm that would be amenable to rigorous mathematical analysis and that would at least w.p.p. produce a 3-colouring for 5-regular graphs. These attempts also failed.

Both the above failures were given a well founded empirical explanation by work in physics. Building on a statistical mechanics analysis of the space of truth assignments of the 3-SAT problem, which has not been shown yet to be mathematically rigorous, and on the Survey Propagation (SP) algorithm for 3-SAT inspired by this analysis (see e.g. [9] and the references therein), Krząkała et al. [8] provided strong evidence that 5-regular graphs are a.a.s. 3-colourable by an SP algorithm. They also showed that the space of assignments of three colours to the vertices (legal or not, i.e. with no two adjacent vertices with the same colour or not) consists of clusters of *legal* colour assignments inside which one can move from point to point by steps of small Hamming distance. However, to go from one cluster to another by such small steps, it is necessary to go through assignments of colours that grossly violate the requirement of legality (high-energy colour assignments). Also, the number of clusters that contain points with energy that is a local, but not global, minimum is exponentially large. As a result, local search algorithms are easily trapped into such local minima (metastable states).

In this article we reduce the problem of proving that random 5-regular graphs are a.a.s. 3-colourable to a problem of a totally different nature, involving simply showing that the maximum of a given function on a given bounded domain occurs at a given location. (In addition we describe extensive calculations which strongly support the hypothesis that the maximum does occur at the given location.) To achieve this, we study locally rainbow balanced colourings of a 5-regular graph, where a colouring is *balanced* if the number of vertices of each colour is equal, and *locally rainbow* if every vertex is adjacent to vertices of all the other colours. We compute the expectation $\mathbf{E}Y$ and variance σ^2 of the number Y of such colourings asymptotically. Assuming a hypothesis stated below, we prove that σ^2 is asymptotically a constant times $(\mathbf{E}Y)^2$. A standard second moment inequality states that Y is nonzero with probability at least $(\mathbf{E}Y)^2/(\mathbf{E}Y^2)$, which is hence bounded away from 0. Instead of this result, we obtain the stronger result, that Y is a.a.s. nonzero, by using the small subgraph conditioning method (see [17]). Previous applications of this method have almost all been to cases where the random variable Y counts subgraphs of some type, usually regular spanning subgraphs. Just a few cases have applied it to other random variables, beginning with numbers of independent sets [4]. The application in the present paper has a more significant consequence.

The reason behind the choice of this particular subset of colourings (balanced and locally rainbow) is that our approach does not work when applied to the full set of colourings. In fact, the second moment of the number of ordinary 3-colourings grows large exponentially faster than the square of its expectation (see the last section in [3]). Restricting the analysis to locally rainbow colourings makes the expectation smaller but fortunately the second moment is decreased even further and the requirements of our method are met. The extra condition that colourings are balanced just makes the computations simpler.

For our calculations, we use the well-known *pairing* or *configuration model* $\mathcal{P}_{n,d}$ which was first introduced by Bollobás [5]. A *pairing* in $\mathcal{P}_{n,d}$ is a perfect matching on a set of dn points which are grouped into n cells of d points each. A random pairing naturally corresponds in an obvious way to a random d-regular multigraph (possibly containing loops or multiple edges), in which each cell becomes a vertex. Colourings of the multigraph then correspond to assignments of colours to the cells of the model. The reader should refer to [17] for aspects of the pairing model not explained here.

The application of the small subgraph conditioning method calls for the computation of joint moments of the numbers of locally rainbow balanced 3-colourings and short cycles. It also requires an upper bound on the second moment of Y, the number of locally rainbow balanced 3-colourings of the random 5-regular pairing $\mathcal{P}_{n,5}$. The estimation of the second moment amounts essentially to counting the number of *pairs* of such colourings on 5-regular graphs. To give an exact expression for $\mathbf{E}(Y^2)$ we had to sum over a large number of variables (9×36). These variables express the number of vertices that have a given pair of colours (out of the nine possible pairs) and also have a given distribution of their five edges with respect to the pair of colours on the other endpoint of these edges. (As we will see there are 36 possible distributions.) The computation of the asymptotic value of this expression (even within a polynomial factor) entails the computation of the global maximum of a function of 9×36 variables. In Section 5 we show how to reduce this computation to the computation of the maximum of a four-variable continuous function F defined over a closed and bounded convex domain. As the definitions of F and its domain are technically involved, we postpone presenting them until Section 5, at which point the motivation behind the technicalities becomes clearer. For the sake of easy reference, we repeat these definitions, and also give an equivalent definition of F, in Section 7.

Regarding the maximization of F, we show that the boundary of its domain contains no local maximizer and that the point $(1/9, 1/9, 1/9, 1/9)$ in the interior of its domain is a local maximizer (by showing that the Hessian of $\ln F$ is negative definite at this point). Although the definition of F involves another function with hundreds of variables, we are able to obtain information on its values by a rather roundabout route. By numerically computing its value at a huge number of locations over a fine grid of its domain, we obtain strong numerical evidence for the following.

Hypothesis 1.1 (Maximum Hypothesis) *The four-variable function $F(\mathbf{n})$ has a unique global maximum over its domain at the point* $(1/9, 1/9, 1/9, 1/9)$.

We point out that for the case of the ordinary (not balanced locally rainbow) colourings there exists an analogue to function F which also has a local maximum at the point $(1/9, 1/9, 1/9, 1/9)$ but unfortunately this is not the global maximum. Provided that the Maximum Hypothesis holds, we can establish the chromatic number of the random 5-regular graph a.a.s.

Theorem 1.1 *Under the Maximum Hypothesis, the chromatic number of $\mathcal{G}_{n,5}$ is a.a.s. 3.*

Thus, we have reduced the problem of proving that $\mathcal{G}_{n,5}$ a.a.s. has chromatic number 3, to showing that the maximum of a smooth function in a bounded domain occurs at the very place that numerical calculations suggest.

In the rest of this article we prove Theorem 1.1 and describe why we are convinced that the function has its maximum at the required location. In Section 2 we explain the small subgraph conditioning method and show how it is used to prove Theorem 1.1 in the case that n is divisible by 6, using the relevant result from [17]. This assumes the results of certain calculations that are performed in Sections 3 to 5. In Section 3 we compute joint moments of the numbers of locally rainbow balanced 3-colourings and short cycles. We develop an exact expression for the second moment $\mathbf{E}(Y^2)$ in Section 4 and determine its asymptotic value, under the Maximum Hypothesis, in Section 5. The argument for n not divisible by 6 is supplied in Section 6. Finally, in Section 7 we present the empirical validation of the Maximum Hypothesis.

2 Small subgraph conditioning

The small subgraph conditioning method was introduced by Robinson and the last author [12, 13]. See [7, Chapter 9] and [17] for a full exposition.

The setting for the method is as follows. A random variable, Y, counts occurrences of some structure, and depends on a parameter n which tends to ∞. The expectation $\mathbf{E}Y$ tends to infinity, and we want to show that $\mathbf{P}(Y>0)\to 1$. The small subgraph conditioning method applies when the variance of Y is of the same order as $(\mathbf{E}Y)^2$. The main computation required is the asymptotic value of some joint moments of the numbers of certain small subgraphs and the random variable Y. The result which the method depends on can be stated as follows (a consequence of [17, Corollary 4.2]). (We use $[x]_m := x(x-1)\cdots(x-m+1)$ to denote falling factorials.)

Theorem 2.1 *Let $\lambda_k>0$ and $\delta_k\geq -1$ be real numbers for $k=1,2,\ldots$ and suppose that for each n there are random variables $X_k=X_k(n)$, $k=1,2,\ldots$ and $Y=Y(n)$, all defined on the same probability space $\mathcal{G}=\mathcal{G}_n$ such that X_k is nonnegative integer valued, Y is nonnegative and $\mathbf{E}Y>0$ (for n sufficiently large). Suppose furthermore that*

(i) For each $j\geq 1$, the variables $X_1,\ldots,X_j$ are asymptotically independent Poisson random variables with $\mathbf{E}X_k\to\lambda_k$,

(ii) if $\mu_k=\lambda_k(1+\delta_k)$, then

$$\frac{\mathbf{E}(Y[X_1]_{m_1}\cdots[X_j]_{m_j})}{\mathbf{E}Y}\to\prod_{k=1}^{j}\mu_k^{m_k} \tag{2.1}$$

for every finite sequence $m_1,\ldots,m_j$ of nonnegative integers,

(iii) $\sum_k \lambda_k\,{\delta_k}^2<\infty$,

(iv) $\mathbf{E}(Y^2)/(\mathbf{E}Y)^2\leq \exp(\sum_k\lambda_k\,{\delta_k}^2)+o(1)$ as $n\to\infty$.

Then $\mathbf{P}(Y>0\mid\mathcal{E})\to 1$, where $\mathcal{E}$ is the event $\wedge_{\delta_k=-1}\{X_k=0\}$.

Proof of Theorem 1.1 (for n divisible by 6) For the application in the present article we use the probability space $\mathcal{G}_n=\mathcal{P}_{n,5}$ with Y counting the number of locally rainbow balanced 3-colourings and X_k counting the number of k-cycles for fixed $k\geq 1$. We assume from now until the very end of this proof that n is divisible by 6. We next discuss how the four conditions of Theorem 2.1 are verified in this setting.

It is well-known (e.g., see [17]) that condition (i) is satisfied by $\lambda_k=4^k/(2k)$. In (3.1) and (3.2) we will see that condition (ii) holds for the function

$$\delta_k=15^{-k}+2(-5)^{-k}+2(-3)^{-k}. \tag{2.2}$$

Substituting this function into conditions (iii) and (iv), we see that the sum is

$$\begin{aligned}\sum_k\lambda_k\delta_k^2 &= \sum_k\frac{(5-1)^k}{2k}\left(15^{-k}+2(-5)^{-k}+2(-3)^{-k}\right)^2\\ &= \sum_k\frac{1}{2k}\left(\left(\frac{4}{225}\right)^k+4\left(\frac{-4}{45}\right)^k+4\left(\frac{-4}{75}\right)^k+4\left(\frac{4}{9}\right)^k+8\left(\frac{4}{15}\right)^k+4\left(\frac{4}{25}\right)^k\right).\end{aligned}$$

Using the identity $\sum_k \frac{1}{2k} x^k = \frac{-1}{2}\ln(1-x)$, this sum becomes

$$\begin{aligned}\sum_k \lambda_k \delta_k^2 &= \frac{-1}{2}\ln\left(\left(\frac{221}{225}\right)\left(\frac{49}{45}\right)^4\left(\frac{79}{75}\right)^4\left(\frac{5}{9}\right)^4\left(\frac{11}{15}\right)^8\left(\frac{21}{25}\right)^4\right) \\ &= \ln\left(\frac{3^{13}5^{13}}{7^6 11^4 79^2\sqrt{13\cdot 17}}\right). \qquad (2.3)\end{aligned}$$

To verify condition (iv), we will need the asymptotic values of the first and second moments of Y. Later in this article we will prove that

$$\mathbf{E}Y \sim \sqrt{\frac{2^2 3^6 5^3}{11^3}\frac{1}{(2\pi n)^2}\left(\frac{25}{24}\right)^n} \qquad (2.4)$$

and, under the Maximum Hypothesis,

$$\mathbf{E}(Y^2) \sim \frac{2^2 3^{19} 5^{16}}{7^6 11^7 79^2\sqrt{13\cdot 17}}\frac{1}{(2\pi n)^2}\left(\frac{25}{24}\right)^n. \qquad (2.5)$$

We compute the ratio

$$\frac{\mathbf{E}(Y^2)}{(\mathbf{E}Y)^2} \sim \frac{3^{13}5^{13}}{7^6 11^4 79^2\sqrt{13\cdot 17}},$$

which matches (2.3), establishing condition (iv). Having verified the four conditions, we may apply the small subgraph conditioning method to conclude $\mathbf{P}(Y>0 \mid \mathcal{E}) \to 1$, where $\mathcal{E}$ is the event $\wedge_{\delta_k=-1}\{X_k=0\}$.

To interpret the event $\mathcal{E}$ in the conclusion, we note that $\delta_1 = -1$ and for $k \geq 2$ we have

$$\begin{aligned}|\delta_k| &\leq 15^{-2} + 2(5)^{-2} + 2(3)^{-2} \\ &< 1.\end{aligned}$$

So the conclusion reads $\mathbf{P}\left(Y>0 \mid X_1 = 0\right) \to 1$. Because $\mathbf{P}\left(X_2 = 0\right)$ is bounded away from 0 for large n, it follows that $Y>0$ a.a.s. for the simple graphs $\mathcal{G}_{n,5}$. This proves Theorem 1.1 provided that n is divisible by 6. ∎

The cases that n is 2 or 4 mod 6 are treated in Section 6. This is done by modifying certain parts of the argument for $n \equiv 0 \pmod 6$ to handle a small number of precoloured vertices, and then applying an asymptotic equivalence between random graph spaces.

3 Joint moments

The goal of this section is to compute asymptotic values of some joint moments for the random variables which count locally rainbow balanced 3-colourings and short cycles in random regular graphs.

On the space $\mathcal{P}_{n,5}$, let Y be the random variable counting the number of locally rainbow balanced 3-colourings. We begin by computing the asymptotic value of $\mathbf{E}Y$.

Lemma 3.1

$$\mathbf{E}Y \sim \binom{n}{n/3, n/3, n/3} \frac{(5n/6)!^3}{|\mathcal{P}_{n,5}|} A(n)$$

where

$$A(n) = \left(\frac{3\sqrt{2}}{\sqrt{11\pi n}} 30^{n/3} \right)^3 .$$

Proof. To compute this expected value we must count, for each of the $\binom{n}{n/3,n/3,n/3}$ ways to assign vertices to equal-sized colour classes, the number of pairings which make the colouring locally rainbow and balanced. All these assignments are equivalent, so fix one of them. Because the three colour classes have equal size, the number of edges between any two colours classes must be $5n/6$. In our discussion, the points in a vertex inherit the colour of that vertex.

To count the pairings which make the colouring locally rainbow and balanced we proceed in two steps. First, at each vertex v, we choose for each point in v the colour of the point it is paired with. This must be done carefully to ensure that each vertex will be adjacent to at least two colours and that the number of edges between the colour classes will be $5n/6$ as required. Then, for each pair of colour classes, we pair up the appropriate points between these classes in one of $(5n/6)!$ ways. Thus, the second step gives us a factor of $(5n/6)!^3$.

To determine the number of choices in the first step, we observe that each colour class produces an equivalent contribution. We fix one colour class, say colour 1, and construct the ordinary generating function which counts the number of ways of choosing the colour of the neighbour of each point within the class, with the indeterminate x marking one of the two possible colours. At each vertex, each of the 5 points can be assigned a mate (i.e. the other point in its pair) of either one of the two colours, provided that not all of the points are assigned to the same colour. Thus the contribution of each vertex to the generating function is $(x+1)^5 - x^5 - 1$, giving us the generating function

$$\left((x+1)^5 - x^5 - 1\right)^{n/3} .$$

Exactly $5n/6$ of these choices must be for the colour marked by x, so the total number of choices for the first step is (letting square brackets denote extraction of a coefficient)

$$N = [x^{5n/6}] \left((x+1)^5 - x^5 - 1\right)^{n/3}$$

for each colour class. Combining these results, we have

$$\mathbf{E}Y = \binom{n}{n/3, n/3, n/3} \frac{(5n/6)!^3}{|\mathcal{P}_{n,5}|} N^3.$$

Using the saddle-point method (see e.g. Section 12.1 in [11]) we will estimate N using a contour integral along the path $|z| = 1$. We begin by substituting $z = \exp(i\theta)$ and expanding in θ.

$$\begin{aligned}
N &= \frac{1}{2\pi i}\int_{|z|=1}\frac{\left((z+1)^5 - z^5 - 1\right)^{n/3}}{z^{5n/6}}dz \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\theta 5n/6}\left((e^{i\theta}+1)^5 - e^{i\theta 5} - 1\right)^{n/3} d\theta \\
&= \frac{1}{2\pi}(2^5-2)^{n/3}\int_{-\pi}^{\pi}\exp\left(-\frac{4^5+4(5)-(5+1)2^{1+5}}{24(2^5-2)^2}n\theta^2 + O(n\theta^3)\right) d\theta \\
&= \frac{1}{2\pi}30^{n/3}\int_{-\pi}^{\pi}\exp\left(-\frac{11}{72}n\theta^2 + O(n\theta^3)\right) d\theta.
\end{aligned}$$

For $|\theta| \le n^{-2/5}$, the contribution to the integral is asymptotically

$$\begin{aligned}
I &= \frac{1}{2\pi}30^{n/3}\int_{-\infty}^{\infty}\exp\left(-\frac{11}{72}n\theta^2\right) d\theta \\
&= \frac{1}{2\pi}30^{n/3}\sqrt{\frac{72\pi}{11n}} \\
&= \frac{3\sqrt{2}}{\sqrt{11\pi n}}30^{n/3}.
\end{aligned}$$

For $|\theta| > n^{-2/5}$, the absolute value of $\left((e^{i\theta}+1)^5 - e^{i\theta 5} - 1\right)^{n/3}$ is

$$\begin{aligned}
& |e^{i\theta}|^{n/3}\left|\sum_{j=1}^{5-1}\binom{5}{j}e^{i\theta j}\right|^{n/3} \\
\le\ & \left(2^5 - 4 + |e^{i\theta}+1|\right)^{n/3} \\
\le\ & \left(2^5 - 4 + \sqrt{2+2\cos\left(n^{-2/5}\right)}\right)^{n/3} \\
=\ & \left(30 - \frac{1}{4}n^{-4/5} + O\left(n^{-8/5}\right)\right)^{n/3} \\
=\ & 30^{n/3}\exp\left(\frac{n}{3}\ln\left(1 - \frac{1}{120}n^{-4/5} + O\left(n^{-8/5}\right)\right)\right) \\
=\ & 30^{n/3}\exp\left(-\frac{1}{360}n^{1/5} + O\left(n^{-3/5}\right)\right),
\end{aligned}$$

which is $o(I)$. Therefore the expression for I gives the correct asymptotic estimate for N, which is

$$N \sim \frac{3\sqrt{2}}{\sqrt{11\pi n}}30^{n/3}.$$

Combining this with our above results, we get Lemma 3.1. ∎

From Lemma 3.1 it is easy to deduce the asymptotic value of $\mathbf{E}Y$ as stated in (2.4). Simply substitute $|\mathcal{P}_{n,5}| = (5n)!/(2^{5n/2}(5n/2)!)$ and apply Stirling's formula. We omit the calculations.

We now move closer to our goal of computing joint moments for locally rainbow balanced 3-colourings and short cycles. For fixed $k \geq 1$, let the random variable X_k count the number of k-cycles in $\mathcal{P}_{n,5}$. We will actually work with rooted oriented cycles, which introduces a factor of $2k$ into the counting. It will be helpful to have the following definition. For a rooted oriented cycle in a coloured graph, define its *colour type* to be the sequence of colours on its vertices. To calculate the expected value of YX_k, we will count, for each locally rainbow balanced 3-colouring and each rooted oriented k-cycle, the number of pairings which contain this cycle and respect this colouring.

As before, there are $\binom{n}{n/3,n/3,n/3}$ ways to choose the balanced 3-colouring. All are equivalent, so fix one. To enumerate the cycles and pairings which respect this colouring, we will sum over all colour types T. Once a colour type has been chosen, each vertex of the cycle can be placed in the pairing model by choosing a vertex of the correct colour and an ordered pair of points in that vertex to be used by the cycle. Hence, in total, there are asymptotically $(5 \times 4 \times n/3)^k$ ways to place the rooted oriented cycle in the pairing model. We now have

$$\mathbf{E}(YX_k) \sim \frac{1}{2k}\binom{n}{n/3, n/3, n/3}\left(\frac{20n}{3}\right)^k \frac{1}{|\mathcal{P}_{n,5}|}\sum_T f(T),$$

where $f(T)$ is the number of pairings which respect a fixed colouring and fixed rooted oriented cycle of colour type T and make the colouring locally rainbow.

To estimate the function $f(T)$, we will again fix one colour class j and construct an ordinary generating function. The generating function will count the number of ways of choosing the colour of the neighbour of each point within the class, with the indeterminate x marking one of the two possible colours.

For $j = 1, 2, 3$, let $\alpha_j(T)$ count the number of j-coloured vertices in colour type T whose two neighbours in the cycle have different colours. Let $\alpha'_j(T)$ count the number of j-coloured vertices in colour type T whose two neighbours in the cycle both have the colour marked by x. Let $\alpha''_j(T)$ count the remaining j-coloured vertices in T. We also define $\beta_j(T) = \alpha'_j(T)+\alpha''_j(T)$.

For any vertex through which the cycle does not pass, the contribution to the generating function is, as before, $(x+1)^5 - x^5 - 1$. For a cycle vertex whose neighbours in the cycle have different colours, we can assign the neighbour colours for the remaining points in any way, giving us $(x+1)^3$. But for a cycle vertex whose neighbours in the cycle have the same colour, we must ensure that this vertex gets at least one neighbour of a different colour so that the colouring is locally rainbow. This gives us $(x+1)^3 - x^3$ if the neighbours have the colour marked by x, and $(x+1)^3 - 1$ otherwise. Combining these functions, the number of ways of choosing the neighbour of each point within colour class j is given by the coefficient of $x^{5n/6}$ in the expression

$$\left((x+1)^5 - x^5 - 1\right)^{n/3-\alpha_j(T)-\alpha'_j(T)-\alpha''_j(T)} \left((x+1)^3\right)^{\alpha_j(T)} \left((x+1)^3 - x^3\right)^{\alpha'_j(T)} \left((x+1)^3 - 1\right)^{\alpha''_j(T)}.$$

Earlier in this section we used the saddle-point method to estimate a similar coefficient. A simple comparison with that previous application makes it easy to see that the current coefficient is asymptotically

$$\frac{30^{n/3-\alpha_j(T)-\beta_j(T)}8^{\alpha_j(T)}7^{\beta_j(T)}3\sqrt{2}}{\sqrt{11\pi n}}.$$

After the colour of the neighbour of each point has been chosen, it remains to pair up the points between each two colour classes. Since the k pairs in the cycle have already been chosen, the number of ways to do this is asymptotically

$$\frac{(5n/6)!^3}{(5n/6)^k}.$$

Putting $\alpha(T) = \alpha_1(T) + \alpha_2(T) + \alpha_3(T)$ and $\beta(T) = \beta_1(T) + \beta_2(T) + \beta_3(T)$, we conclude that

$$\begin{aligned} f(T) &\sim \frac{30^{n-\alpha(T)-\beta(T)}8^{\alpha(T)}7^{\beta(T)}3^3\sqrt{2}^3}{\left(\sqrt{11\pi n}\right)^3} \times \frac{(5n/6)!^3}{(5n/6)^k} \\ &\sim A(n)\frac{(5n/6)!^3}{(5n/6)^k}\left(\frac{8}{30}\right)^{\alpha(T)}\left(\frac{7}{30}\right)^{\beta(T)}. \end{aligned}$$

Letting $c_\alpha = 8/30$ and $c_\beta = 7/30$, it remains to estimate

$$S = \sum_T c_\alpha^{\alpha(T)} c_\beta^{\beta(T)}$$

where the sum is taken over all colour types T. In other words, we need to enumerate the colour types, introducing a factor of c_α for each cycle vertex whose neighbours have different colours, and a factor of c_β for each of the remaining cycle vertices.

It is helpful to view each colour type as a sequence of ordered pairs of colours: the colours at the endpoints of each edge, taken in the order induced by the orientation of cycle. One could consider each possible pair to be a state in a Markov chain. Number the states as follows.

state	pair of colours
1	12
2	21
3	31
4	13
5	23
6	32

Each colour type on k vertices then corresponds to a sequence of $k+1$ states where the first state equals the last state. For example, consider the colour type with colour sequence $1, 2, 3, 2$. It corresponds to the state sequence $1, 5, 6, 2, 1$. The transition from state 1 to state 5 represents to a vertex (of colour 2) whose neighbours in the cycle have different colours (1 and 3); hence it should introduce a factor of c_α. Thus, in the matrix below, the entry at position $(1, 5)$ is c_α. In this way we can construct a matrix which accounts for all possible transitions, and use it to obtain the desired enumeration. The above sum S equals $\mathrm{Tr}(M^k)$, where Tr denotes the trace, and M is the "transition" matrix

$$\begin{bmatrix} 0 & c_\beta & 0 & 0 & c_\alpha & 0 \\ c_\beta & 0 & 0 & c_\alpha & 0 & 0 \\ c_\alpha & 0 & 0 & c_\beta & 0 & 0 \\ 0 & 0 & c_\beta & 0 & 0 & c_\alpha \\ 0 & 0 & c_\alpha & 0 & 0 & c_\beta \\ 0 & c_\alpha & 0 & 0 & c_\beta & 0 \end{bmatrix}.$$

The eigenvalues of this matrix are $c_\beta + c_\alpha$, $-c_\beta + c_\alpha$, $-\frac{1}{2}c_\alpha + \frac{1}{2}\sqrt{-3c_\alpha^2 + 4c_\beta^2}$, and $-\frac{1}{2}c_\alpha - \frac{1}{2}\sqrt{-3c_\alpha^2 + 4c_\beta^2}$. The last two eigenvalues have multiplicity 2. Thus

$$\begin{aligned} S = (c_\beta + c_\alpha)^k \quad & + \quad (-c_\beta + c_\alpha)^k \\ & + \quad 2\left(-\frac{1}{2}c_\alpha + \frac{1}{2}\sqrt{-3c_\alpha^2 + 4c_\beta^2}\right)^k \\ & + \quad 2\left(-\frac{1}{2}c_\alpha - \frac{1}{2}\sqrt{-3c_\alpha^2 + 4c_\beta^2}\right)^k . \end{aligned}$$

Since $c_\beta + c_\alpha = 7/30 + 8/30 = 1/2$, we may write

$$S = \frac{1}{2^k}\left(1 + \delta_k\right)$$

where

$$\delta_k = 15^{-k} + 2(-5)^{-k} + 2(-3)^{-k} \tag{3.1}$$

which is (2.2).

We conclude that

$$\mathbf{E}(YX_k) \sim \frac{1}{2k}\binom{n}{n/3, n/3, n/3}\left(\frac{20n}{3}\right)^k \frac{1}{|\mathcal{P}_{n,5}|} A(n) \frac{(5n/6)!^3}{(5n/6)^k} S,$$

and hence, combining this result with the previous lemma,

$$\begin{aligned} \frac{\mathbf{E}(YX_k)}{\mathbf{E}Y} & \sim \frac{1}{2k} 8^k S \\ & \sim \frac{4^k}{2k}\left(1 + \delta_k\right). \end{aligned}$$

The above argument is easily extended to work for higher moments, by counting the pairings that contain a given locally rainbow balanced 3-colouring and set of oriented cycles of the appropriate lengths. The contribution from cases where the cycles intersect turn out to be negligible, for the following reasons. Suppose that the cycles form a subgraph H with ν

vertices and μ edges, and the total length of cycles is ν_0. Then in the case of disjoint cycles, $\nu = \mu = \nu_0$. A factor of $\Theta(n^{\nu-\nu_0})$ is lost if there is a reduction in the number of vertices of H, compared with the disjoint case, because of the reduced number of ways of placing the cycles on the coloured vertices. Similarly, a factor $\Theta(n^{\nu_0-\mu})$ is gained in the function f for the reduction in the number of edges of H, because of the corresponding increase in the number of points to be paired up at the end. Thus, the contribution from such an arrangement of cycles to the quantity being estimated is of the order of $n^{\nu-\mu}$ times that of the contribution from disjoint cycles. In all non-disjoint cases, H has more edges than vertices, since its minimum degree is at least 2, and it has at least one vertex of degree at least 3. There are only finitely many isomorphism types of H to consider, so the contribution from the case of disjoint cycles is of the order of n times the rest. The significant terms in this case decompose into a product of the factors corresponding to the individual cycles. Consequently, we obtain the following result, as required for (2.1) in accordance with (2.2):

$$\frac{\mathbf{E}(Y[X_1]_{m_1}\cdots[X_j]_{m_j})}{\mathbf{E}Y} \sim \prod_{k=1}^{j}\left(\frac{4^k}{2k}\left(1+\delta_k\right)\right)^{m_k}. \tag{3.2}$$

4 Exact Expression for the Second Moment

Given a pairing $P \in \mathcal{P}_{n,5}$, let $\mathcal{R}_P$ be the class of locally rainbow balanced 3-colourings of P. Let Y be the random variable that counts the number of locally rainbow balanced 3-colourings in $\mathcal{P}_{n,5}$. Then, it is easily shown that

$$\mathbf{E}(Y^2) = \frac{|\{(P, C_1, C_2) \mid P \in \mathcal{P}_{n,5}, C_1, C_2 \in \mathcal{R}_P\}|}{|\mathcal{P}_{n,5}|}. \tag{4.1}$$

Below we assume we are given a pairing P and two locally rainbow balanced 3-colourings C_1 and C_2 on P. Recall that a pairing is a perfect matching on $5n$ points which are organized into n cells of 5 points each. For $i, j = 0, 1, 2$, let $V^{i,j}$ be the set of cells coloured with i and j with respect to colourings C_1 and C_2, respectively. Let $n^{i,j} = |V^{i,j}|/n$ and let $E^{i,j}$ be the set of points in cells of $V^{i,j}$. Since C_1 and C_2 are balanced, we have

$$\sum_i n^{i,j} = 1/3,\ \forall j, \quad \sum_j n^{i,j} = 1/3,\ \forall i, \tag{4.2}$$

and therefore $\sum_{i,j} n^{i,j} = 1$. Also, for $r, t \in \{-1, 1\}$, let $E^{i,j}_{r,t}$ be the set of points in $E^{i,j}$ which are matched with points in $E^{i+r,j+t}$. (Here and throughout the article, the arithmetic in the indices is modulo 3.) Let $m^{i,j}_{r,t} = |E^{i,j}_{r,t}|/n$. For fixed i and j, it is convenient to think of the four variables $(m^{i,j}_{r,t})_{r,t\in\{-1,1\}}$ as the entries of a 2×2 matrix. The rows and columns are indexed by -1 and 1, with -1 for the first row or column. We have that $\sum_{r,t} m^{i,j}_{r,t} = 5n^{i,j}$, and therefore $\sum_{i,j,r,t} m^{i,j}_{r,t} = 5$. And, since matching sets of points should have equal cardinalities, we also have that

$$m^{i,j}_{r,t} = m^{i+r,j+t}_{-r,-t}. \tag{4.3}$$

Let v be a cell in $V^{i,j}$. The *spectrum* s of cell v is a 2×2 nonnegative integer matrix. The rows and columns are indexed by -1 and 1, with -1 for the first row or column. Cell v is said to have spectrum s if $s_{r,t}$ out of its five points, $r,t\in\{-1,1\}$, are matched to points in cells of $V^{i+r,j+t}$. The sum of the entries of s is 5 because of the 5-regularity of the graph. Each row and column sum is at least 1 because both C_1 and C_2 are locally rainbow. We let $\mathcal{S}$ denote the set of possible spectra. One can check that $|\mathcal{S}|=36$.

For each $i,j\in\mathbb{Z}_3$ and spectrum $s\in\mathcal{S}$, we denote by $d_s^{i,j}$ the scaled (with respect to n) number of cells which belong to $V^{i,j}$ and have spectrum s. We have

$$m^{i,j}=\sum_{s\in\mathcal{S}} d_s^{i,j}\, s, \tag{4.4}$$

$$n^{i,j}=\sum_{s\in\mathcal{S}} d_s^{i,j}, \tag{4.5}$$

and therefore $\sum_{i,j,s} d_s^{i,j}=1$.

Throughout this paper we refer to the set of the nine numbers $n^{i,j}$ as the set of the *overlap variables*. We also refer to the set of the thirty-six numbers $m_{r,t}^{i,j}$ as the set of the *matching variables*. We refer to the 9×36 numbers $d_s^{i,j}$ as the *spectral variables*.

We consider the polytope

$$\begin{aligned}\mathcal{D}=\ &\Big\{(d_s^{i,j})_{i,j\in\mathbb{Z}_3,s\in\mathcal{S}}\in\mathbb{R}^{324}\ :\ d_s^{i,j}\geq 0\ \forall i,j,s,\ \textstyle\sum_{j,s} d_s^{i,j}=\frac{1}{3}\ \forall i,\\ &\textstyle\sum_{i,s} d_s^{i,j}=\frac{1}{3}\ \forall j,\ \sum_s s_{r,t}d_s^{i,j}=\sum_s s_{-r,-t}d_s^{i+r,j+t}\ \forall i,j,r,t\Big\},\end{aligned}$$

and the discrete subset

$$\mathcal{I}=\mathcal{D}\cap\left(\frac{1}{n}\mathbb{Z}^{324}\right).$$

In view of (4.2)–(4.5), note that $\mathcal{I}$ contains the set of sequences $(d_s^{i,j})_{i,j\in\mathbb{Z}_3,s\in\mathcal{S}}$ that correspond to some pair of locally rainbow balanced 3-colourings. Given a fixed sequence $(d_s^{i,j})\in\mathcal{I}$, let us denote by $\binom{n}{(d_s^{i,j}n)}$ the multinomial coefficient that counts the number of ways to distribute the n vertices into classes of cardinality $d_s^{i,j}n$ for all possible values of i,j and s. Define $m^{i,j}$ by (4.4). Also let $\binom{5}{s}$ stand for $5!/\prod_{r,t}s_{r,t}!$.

Let $N=|\{(P,C_1,C_2)\mid P\in\mathcal{P}_{n,5},C_1,C_2\in\mathcal{R}_P\}|$. By counting the ways to assign spectra to cells, and then colours to points in cells given their spectra, and finally the number of matchings between colour classes, we have

$$N=\sum_{\mathcal{I}}\left\{\binom{n}{(d_s^{i,j}n)}\left(\prod_{i,j,s}\binom{5}{s}^{d_s^{i,j}n}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)\right\}. \tag{4.6}$$

Dividing this by $|\mathcal{P}_{n,5}|=(5n)!/(2^{5n/2}(5n/2)!)$, we obtain

$$\mathbf{E}(Y^2)=\frac{2^{5n/2}(5n/2)!}{(5n)!}\sum_{\mathcal{I}}\left\{\binom{n}{(d_s^{i,j}n)}\left(\prod_{i,j,s}\binom{5}{s}^{d_s^{i,j}n}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)\right\}. \tag{4.7}$$

5 Asymptotic Value of $\mathbf{E}(Y^2)$

In this section, we complete the proof of the main theorem given in Section 2 by showing that equation (2.5) holds, assuming the Maximum Hypothesis.

For sake of simplicity, we will often write $\mathbf{d}$ to denote the tuple $(d_s^{i,j})_{i,j\in\mathbb{Z}_3,s\in\mathcal{S}}$. Let us consider the function

$$\hat{F}(\mathbf{d}) = \left(\prod_{i,j,s}\left(\frac{\binom{5}{s}}{d_s^{i,j}}\right)^{d_s^{i,j}}\right)\left(\prod_{i,j,r,t}\left(m_{r,t}^{i,j}\right)^{\frac{1}{2}m_{r,t}^{i,j}}\right),$$

defined in $\mathcal{D}$, where $m_{r,t}^{i,j}$ denotes $\sum_s s_{r,t}d_s^{i,j}$ as before. Throughout this article we observe the conventions that $0^0 = 1$ and $0\ln 0 = 0$.

We define

$$f(\mathbf{d}) = \ln\hat{F}(\mathbf{d}) = \sum_{i,j,s} d_s^{i,j}\left(\ln\binom{5}{s} - \ln d_s^{i,j}\right) + \sum_{i,j,r,t}\frac{1}{2}m_{r,t}^{i,j}\ln m_{r,t}^{i,j},$$

$$g(\mathbf{d}) = \frac{\prod_{i,j,r,t}\left(m_{r,t}^{i,j}\right)^{1/4}}{\prod_{i,j,s}(d_s^{i,j})^{1/2}}, \qquad h(n) = 2^{-1/2}(2\pi n)^{-305/2}\,5^{-5n/2}. \tag{5.1}$$

Lemma 5.1 *The second moment satisfies*

$$\mathbf{E}(Y^2) = h(n)\sum_{\mathbf{d}\in\mathcal{I}} q(n,\mathbf{d})e^{f(\mathbf{d})n} \tag{5.2}$$

where, as $n\to\infty$ and uniformly over all $\mathbf{d}$, $q(n,\mathbf{d}) = O(n^{162})$ and $q(n,\mathbf{d})\sim g(\mathbf{d})$ provided all $d_s^{i,j}$ and $m_{r,t}^{i,j}$ are bounded away from 0.

Proof. We apply Stirling's formula and perform simple manipulations to (4.7) to obtain:

$$\begin{aligned}
\mathbf{E}(Y^2) \quad &= \frac{2^{5n/2}(5n/2)!n!}{(5n)!}\sum_{\mathbf{d}\in\mathcal{I}}\left\{\left(\prod_{i,j,s}\frac{\binom{5}{s}^{d_s^{i,j}n}}{(d_s^{i,j}n)!}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)\right\}\\
&\sim \sqrt{\pi n}\,5^{-5n/2}\sum_{\mathbf{d}\in\mathcal{I}}\left\{\frac{(n/e)^n}{(n/e)^{5n/2}}\left(\prod_{i,j,s}\frac{\binom{5}{s}^{d_s^{i,j}n}}{(d_s^{i,j}n)!}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)\right\}\\
&= h(n)\sum_{\mathbf{d}\in\mathcal{I}}\left\{\frac{(2\pi n)^{153}(n/e)^n}{(n/e)^{5n/2}}\left(\prod_{i,j,s}\frac{\binom{5}{s}^{d_s^{i,j}n}}{(d_s^{i,j}n)!}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)\right\}.
\end{aligned} \tag{5.3}$$

Now we need to uniformly approximate the factorial of several numbers not necesarily growing large with n. Stirling's formula also implies $k! = \sqrt{2\pi\eta(k)}(k/e)^k$ for all $k\geq 0$, where $\eta(k)\sim k$ if $k\to\infty$, and $\eta(k) = \Theta(k+1)$ for all $k\geq 0$. (In particular, η is nonzero.) So we have

$$\left(\prod_{i,j,s}\frac{\binom{5}{s}^{d_s^{i,j}n}}{(d_s^{i,j}n)!}\right)\left(\prod_{i,j,r,t}\left((m_{r,t}^{i,j}n)!\right)^{1/2}\right)$$

$$= \left(\prod_{i,j,s} \frac{\binom{5}{s}^{d_s^{i,j}n}}{\sqrt{2\pi\eta(d_s^{i,j}n)}\left(\frac{d_s^{i,j}n}{e}\right)^{d_s^{i,j}n}} \right) \left(\prod_{i,j,r,t} \left(\sqrt{2\pi\eta(m_{r,t}^{i,j}n)} \left(\frac{m_{r,t}^{i,j}n}{e}\right)^{m_{r,t}^{i,j}n} \right) \right)^{1/2}$$

$$= \frac{(n/e)^{5n/2}}{(2\pi n)^{153}(n/e)^n} \frac{\prod_{i,j,r,t}(\eta(nm_{r,t}^{i,j})^{1/4}n^{-1/4})}{\prod_{i,j,s}(\eta(nd_s^{i,j})^{1/2}n^{-1/2})} \left(\prod_{i,j,s} \left(\frac{\binom{5}{s}}{d_s^{i,j}} \right)^{d_s^{i,j}n} \right) \left(\prod_{i,j,r,t} (m_{r,t}^{i,j})^{m_{r,t}^{i,j}n/2} \right)$$

$$= \frac{(n/e)^{5n/2}}{(2\pi n)^{153}(n/e)^n} q(n,\mathbf{d})e^{f(\mathbf{d})n}$$

for a function q of the type in the statement of the lemma. Combining this with (5.3) yields the statement of the lemma. ∎

Notice that the number of terms in (5.2) is at most $(n+1)^{324}$, since each coordinate of any $\mathbf{d} \in \mathcal{I}$ must be a rational in $\frac{1}{n}\mathbb{Z}$ between 0 and 1. We consider the maximum base of the exponential part of the terms in (5.2), taken over all points in the polytope $\mathcal{D}$:

$$M = \max_{\mathbf{d}\in\mathcal{D}} \left\{ 5^{-5/2} e^{f(\mathbf{d})} \right\}.$$

This is well defined, due to the compactness of the domain and the continuity of the expression. Note that the exponential behavior of the second moment is governed by M since the number of terms in the sum in (5.2) is polynomial with respect to n.

In the next subsection we determine the value of M under the Maximum Hypothesis. In the following subsection, based on that fact and using a Laplace-type integration argument, we compute the sub-exponential factors in the asymptotic expression of the second moment, and obtain (2.5).

5.1 Computing M

We will maximize $\hat{F}$ in two phases. In the first one, we will maximize $\hat{F}$ assuming the matching variables $m_{r,t}^{i,j}$ are fixed constants. These constants must be compatible with the polytope $\mathcal{D}$ over which $\hat{F}$ is defined, so we define $\mathcal{M}$ to be the set of vectors $\mathbf{m}$ of 2×2 matrices $(m^{i,j})_{i,j\in\mathbb{Z}_3}$ such that (4.4) holds for some $\mathbf{d} \in \mathcal{D}$.

We will often consider variables $d_s^{i,j}$ and $m_{r,t}^{i,j}$ for fixed $i,j \in \mathbb{Z}_3$. To simplify notation, we delete the indices i and j when they are fixed throughout the formula. We also define, for any $0 < c \in \mathbb{R}$,

$$\mathcal{D}'(c) = \{(d_s)_{s\in\mathcal{S}} \in \mathbb{R}^{36} \ : \ d_s \geq 0 \ \forall s, \ \sum_s d_s = c\},$$

and let $\mathcal{M}'(c)$ be the set of 2×2 matrices m such that (4.4) holds for some $(d_s)_{s\in\mathcal{S}} \in \mathcal{D}'(c)$ (after deleting superscripts i and j). We will use $\mathbf{d}$ to denote both points in $\mathcal{D}$ and $\mathcal{D}'(c)$. The meaning will be clear from the context.

In order to give an alternative characterization of the matching variables $m_{r,t}^{i,j}$, we consider the following equations for all ordered pairs (i,j), $i,j \in \mathbb{Z}_3$, and all $r,t \in \{-1,1\}$:

$$\begin{array}{rcl} m^{i,j}_{r,t} & \geq & 0, \\ m^{i,j}_{r,t} + m^{i,j}_{r,-t} & \leq & 4(m^{i,j}_{-r,t} + m^{i,j}_{-r,-t}), \\ m^{i,j}_{r,t} + m^{i,j}_{-r,t} & \leq & 4(m^{i,j}_{r,-t} + m^{i,j}_{-r,-t}). \end{array} \tag{5.4}$$

That is, for all such i and j, the entries of $m^{i,j}$ are nonnegative, neither row sum is greater than 4 times the other, and neither column sum is greater than 4 times the other.

Lemma 5.2 *Let $c > 0 \in \mathbb{R}$. The set $\mathcal{M}'(c)$ can be alternatively described as the polytope containing all matrices m such that*

$$\sum_{r,t} m_{r,t} = 5c, \tag{5.5}$$

and the constraints in (5.4) hold. Similarly, $\mathcal{M}$ is the polytope containing all vectors $\mathbf{m}$ of matrices $m^{i,j}$ such that

$$\sum_{i,r,t} m^{i,j}_{r,t} = 5/3, \quad \sum_{j,r,t} m^{i,j}_{r,t} = 5/3, \tag{5.6}$$

and the constraints in (4.3), (5.4) hold.

Proof. Let $\mathcal{A}$ be the set of matrices m satisfying (5.4) and (5.5).
$\mathcal{M}'(c) \subseteq \mathcal{A}$:

Let m be a matrix in $\mathcal{M}'(c)$. Then, for some $\mathbf{d} \in \mathcal{D}'(c)$, we have

$$\sum_{r,t} m_{r,t} = \sum_{r,t} \sum_{s} s_{r,t} d_s = \sum_{s} \sum_{r,t} s_{r,t} d_s = \sum_{s} 5 d_s = 5c,$$

and (5.5) is satisfied. Moreover, we observe that for any spectrum s, we have

$$s_{r,t} \geq 0, \;\; s_{r,t} + s_{r,-t} \leq 4(s_{-r,t} + s_{-r,-t}) \;\text{ and }\; s_{r,t} + s_{-r,t} \leq 4(s_{r,-t} + s_{-r,-t}).$$

Then m must satisfy the constraints in (5.4), since it is a positive linear combination of spectra, and $m \in \mathcal{A}$.
$\mathcal{A} \subseteq \mathcal{M}'(c)$:

$\mathcal{A}$ is a polytope and so it is the convex hull of its vertices:

$$\begin{bmatrix} c & 0 \\ 0 & 4c \end{bmatrix}, \begin{bmatrix} 0 & c \\ c & 3c \end{bmatrix}, \begin{bmatrix} 0 & c \\ 4c & 0 \end{bmatrix}, \begin{bmatrix} c & 0 \\ 3c & c \end{bmatrix}, \begin{bmatrix} 0 & 4c \\ c & 0 \end{bmatrix}, \begin{bmatrix} c & 3c \\ 0 & c \end{bmatrix}, \begin{bmatrix} 4c & 0 \\ 0 & c \end{bmatrix}, \begin{bmatrix} 3c & c \\ c & 0 \end{bmatrix}$$

Each of these vertices v has the shape of some spectrum s times c. By making $d_s = c$ and $d_{s'} = 0$ for $s' \neq s$, we show that $v \in \mathcal{M}'(c)$.

Moreover, we observe that $\mathcal{M}'(c)$ is a convex set, since it is the image of $\mathcal{D}'(c)$ under a linear mapping. Then $\mathcal{M}'(c)$ must contain the convex hull of the vertices of $\mathcal{A}$, and thus $\mathcal{A}$.

The second statement in the lemma follows easily from this and from the definition of $\mathcal{M}$.
∎

For any fixed $\mathbf{m} \in \mathcal{M}$, let $\tilde{F}(\mathbf{m})$ be the maximum of $\hat{F}$ restricted to $\mathbf{d} \in \mathcal{D}$ such that (4.4) holds. To express $\tilde{F}(\mathbf{m})$ in terms of $\mathbf{m}$, we will use the matrix function

$$\begin{aligned}\Phi \begin{bmatrix} x & y \\ z & w \end{bmatrix} &= \sum_{s \in \mathcal{S}} \binom{5}{s} x^{s_{-1,-1}} y^{s_{-1,1}} z^{s_{1,-1}} w^{s_{1,1}} \\ &= (x+y+z+w)^5 - (x+y)^5 - (x+z)^5 \\ &\quad - (y+w)^5 - (z+w)^5 + x^5 + y^5 + z^5 + w^5 \end{aligned} \tag{5.7}$$

and, for each of the nine possible pairs (i,j), $i,j \in \mathbb{Z}_3$, consider the 4×4 system

$$\mu^{i,j}_{r,t} \frac{\partial \; \Phi \mu^{i,j}}{\partial \mu^{i,j}_{r,t}} = m^{i,j}_{r,t}, \qquad r,t = -1, 1, \tag{5.8}$$

in the matrix variables $\mu^{i,j}$.

Lemma 5.3 *For any* $\mathbf{m}$ *in the interior of* $\mathcal{M}$*, each of the nine systems in (5.8) has a unique positive solution. Moreover, in terms of the solutions of these systems,*

$$\tilde{F}(\mathbf{m}) = \prod_{i,j,r,t} \left(\frac{(m^{i,j}_{r,t})^{\frac{1}{2}}}{\mu^{i,j}_{r,t}} \right)^{m^{i,j}_{r,t}},$$

and the equation remains valid for $\mathbf{m}$ *on the boundary of* $\mathcal{M}$ *if the expression on the right is extended by continuity.*

Proof. We assume that $\mathbf{m}$ is a fixed vector in the interior of $\mathcal{M}$. In order to compute $\tilde{F}(\mathbf{m})$, it is sufficient to maximize the function $\hat{F}(\mathbf{d})$ for nonnegative $d^{i,j}_s$ subject to (4.4), since the other constraints are trivially satisfied. We observe that the factor $\prod \left(m^{i,j}_{r,t}\right)^{\frac{1}{2} m^{i,j}_{r,t}}$ is constant, and that variables $d^{i,j}_s$ with different pairs of indices (i,j) appear in different factors of $\hat{F}$ and also in different constraints. Thus, it is sufficient to maximize, separately for each $i,j \in \mathbb{Z}_3$, the function

$$G^{i,j} = \prod_{s \in \mathcal{S}} \left(\frac{\binom{5}{s}}{d^{i,j}_s} \right)^{d^{i,j}_s}, \tag{5.9}$$

over nonnegative $d^{i,j}_s$ subject to the matrix constraint (4.4). From now on in this proof, we fix i and j and thus omit superscripts as discussed above.

Let $\mathcal{R}$ be the polytope containing all $\mathbf{d} = (d_s)_{s \in \mathcal{S}}$ such that d_s is nonnegative for all $s \in \mathcal{S}$, and satisfying (4.4). The fact that $\mathbf{m}$ is in the interior of $\mathcal{M}$ implies that $\mathcal{R}$ contains points with all the d_s strictly positive. In fact, the interior of $\mathcal{R}$ consists of all those points in $\mathcal{R}$ with this property.

For any point $\mathbf{d}_0$ on the boundary of $\mathcal{R}$ we select a segment joining $\mathbf{d}_0$ with some interior point. We observe that, in moving along the segment from the interior of $\mathcal{R}$ towards $\mathbf{d}_0$, the directional derivative of $\ln G$ contains the sum of some bounded terms plus some terms of the type $\ln d_s$ with positive coefficient, which become large as we approach $\mathbf{d}_0$. Hence, G does not maximize at the boundary of $\mathcal{R}$.

We temporarily relax the constraint (4.4) and observe that the Hessian of $\ln G$ is negative definite for any tuple of positive d_s. Hence $\ln G$ is strictly concave in that domain and also in the interior of $\mathcal{R}$, since linear constraints do not affect concavity. Thus, the maximum of G is unique and occurs in the only stationary point of $\ln G$ in the interior of $\mathcal{R}$.

We are now in a good position to apply the Lagrange multipliers method to look for stationary points of $\ln G$. We consider

$$\ln G = \sum_s d_s \left(\ln \binom{5}{s} - \ln d_s \right), \tag{5.10}$$

for positive d_s subject to the four constraints:

$$L_{r,t} = \sum_s s_{r,t} d_s - m_{r,t} = 0, \quad r, t \in \{-1, 1\}. \tag{5.11}$$

For each one of the four constraints $L_{r,t}$ in (5.11) a Lagrange multiplier is $\lambda_{r,t}$ introduced. Then we obtain the following equations:

$$\ln \binom{5}{s} - 1 - \ln d_s = \sum_{r,t} \lambda_{r,t} s_{r,t}, \quad \forall s \in \mathcal{S} \tag{5.12}$$

which, together with the constraints (5.11) have a unique solution when $\mathbf{d}$ is the only stationary point of $\ln G$. Let us define $\mu_{r,t} = \exp(-\lambda_{r,t} - 1/5)$. After exponentiating (5.12), and noting that the sum of the $s_{r,t}$ is 5, we have

$$d_s = \binom{5}{s} \prod_{r,t} (\mu_{r,t})^{s_{r,t}}, \quad \forall s \in \mathcal{S}, \tag{5.13}$$

and combining this with (5.11) gives

$$\begin{aligned} m_{r,t} &= \sum_s \left(s_{r,t} \binom{5}{s} \prod_{r',t'} (\mu_{r',t'})^{s_{r',t'}} \right), \qquad r, t \in \{-1, 1\} \\ &= \mu_{r,t} \frac{\partial}{\partial \mu_{r,t}} \sum_s \left(\binom{5}{s} \prod_{r',t'} (\mu_{r',t'})^{s_{r',t'}} \right), \qquad r, t \in \{-1, 1\}. \end{aligned} \tag{5.14}$$

By construction, this system has a unique positive solution, and (5.13) gives the maximizer of G in terms of this solution. From (5.7), we observe that (5.14) is exactly the same system as the one in (5.8).

Now the maximum of G can be obtained by plugging (5.13) into (5.9), resulting in

$$\max_{\mathbf{d} \in \mathcal{R}} G(\mathbf{d}) = \prod_{r,t} \left(\frac{1}{\mu_{r,t}} \right)^{m_{r,t}}, \tag{5.15}$$

and the required expression for $\tilde{F}(\mathbf{m})$ follows by elementary computations. ∎

Let us now define for any $\mathbf{d} \in \mathcal{D}'(1/9)$ the auxiliary function

$$\hat{G}(\mathbf{d}) = \left(\prod_s \left(\frac{\binom{5}{s}}{d_s} \right)^{d_s} \right) \left(\prod_{r,t} (m_{r,t})^{\frac{1}{2} m_{r,t}} \right), \tag{5.16}$$

where $m_{r,t} = \sum_s s_{r,t}\, d_s$. (Recall that $0^0 = 1$.)

Lemma 5.4 *The function $\hat{G}$ takes its maximum on $\mathcal{D}'(1/9)$ in the interior of $\mathcal{D}'(1/9)$.*

Proof. It is easy to see that the boundary of $\mathcal{D}'(1/9)$ comprises the points where for at least one s, $d_s = 0$ and $\sum_s d_s = 1/9$. We observe that it is sufficient to prove the statement for $\ln \hat{G}$. The continuity of $\ln \hat{G}$ at the boundary points of $\mathcal{D}'(1/9)$ follows from the fact that

$$\lim_{x \to 0} x^x = 1.$$

After proving $\ln \hat{G}$ is continuous at the boundary of $\mathcal{D}'(1/9)$, take any $\mathbf{d}$ on the boundary. Here $d_{s_0} = 0$ for some s_0. Then $d_{s_1} > 0$ for some s_1 since the sum of entries of $\mathbf{d}$ is $1/9$. At any point $\mathbf{d}$ such that $d_s > 0$,

$$\frac{\partial \ln \hat{G}}{\partial d_s} = \ln \binom{5}{s} - 1 - \ln d_s + \frac{5}{2} + \sum_{r,t} \frac{1}{2} s_{r,t} \ln m_{r,t}. \tag{5.17}$$

(Note: if $d_s > 0$ then all the $m_{r,t}$ corresponding to a nonzero $s_{r,t}$ are also necessarily nonzero.)

As a first case, suppose none of the $m_{r,t}$ is zero at $\mathbf{d}$. Then at a point $\mathbf{d} + \epsilon E_{s_0} - \epsilon E_{s_1}$ (here E_s denotes the vector with 1 in its s coordinate and zero elsewhere) $\frac{\partial \ln \hat{G}}{\partial d_{s_0}} - \frac{\partial \ln \hat{G}}{\partial d_{s_1}} \to \infty$ as $\epsilon \to 0$. (Since the first partial goes to ∞ and the second is bounded.) Hence there is no maximum at $\mathbf{d}$.

Next suppose precisely one $m_{r,t}$ is zero at $\mathbf{d}$ (fix such values of r and t). Pick an s such that $s_{r,t} = 1$. Then $d_s = 0$ at $\mathbf{d}$. So rename s as s_0 and use the above argument, choosing again any s_1 with $d_{s_1} > 0$. Now the unbounded terms in $\frac{\partial \ln \hat{G}}{\partial d_{s_0}}$ are $-\ln d_{s_0} + \frac{1}{2}(s_0)_{r,t} \ln m_{r,t}$ and we have $m_{r,t} \geq d_{s_0}$ because $(s_0)_{r,t} = 1$. It follows that there is no maximum at $\mathbf{d}$.

For two different $m_{r,t}$ equal to zero at $\mathbf{d}$, pick the spectrum s_0 to have 1 in one of the corresponding positions, and zero in the other. Then the same argument as above gives the result.

So no local maximum occurs on the boundary. The result follows. ∎

Lemma 5.5 *The function $\hat{G}$ has a unique maximum in $\mathcal{D}'(1/9)$ at the point where all the d_s are equal to $\binom{5}{s}/8100$. The function value at the maximum is $(5^{5/2} 25/24)^{1/9}$.*

Proof. We note that (4.4) maps the interior of $\mathcal{D}'(1/9)$ into the interior of $\mathcal{M}'(1/9)$. As a result and in view of Lemma 5.4, the maximum of $\hat{G}$, under mapping (4.4), does not occur on the boundary of $\mathcal{M}'(1/9)$.

Assume that m is a fixed matrix in the interior of $\mathcal{M}'(1/9)$. We first maximize $\hat{G}$ in $\mathcal{D}'(1/9)$ subject to the matrix constraint (4.4). Denote this maximum by $\tilde{G}(m)$. By arguing as in the proof of Lemma 5.3, we have

$$\tilde{G}(m) = \prod_{r,t} \left(\frac{(m_{r,t})^{\frac{1}{2}}}{\mu_{r,t}} \right)^{m_{r,t}},$$

where the $\mu_{r,t}$ are the unique positive solution of the system in (5.8) after deleting superscripts i and j. Moreover, the maximizer is given in terms of this solution by (5.13).

We now maximize $\tilde{G}$ in the interior of $\mathcal{M}'(1/9)$, by applying the Lagrange multiplier method to

$$\ln \tilde{G}(m) = \sum_{r,t} m_{r,t} \left(\frac{1}{2} \ln m_{r,t} - \ln \mu_{r,t} \right),$$

subject to

$$\sum_{r,t} m_{r,t} = 5/9.$$

We need some preliminary computations. By adding the four equations in (5.8) and taking into account (5.7), we have

$$5\Phi(\mu) = \sum_{r,t} m_{r,t}.$$

In view of this, we have for all $r, t \in \{-1, 1\}$

$$\begin{aligned} \sum_{r',t' \in \{-1,1\}} m_{r',t'} \frac{\partial \ln \mu_{r',t'}}{\partial m_{r,t}} &= \sum_{r',t' \in \{-1,1\}} \frac{m_{r',t'}}{\mu_{r',t'}} \frac{\partial \mu_{r',t'}}{\partial m_{r,t}} = \sum_{r',t' \in \{-1,1\}} \frac{\partial \Phi(\mu)}{\partial \mu_{r',t'}} \frac{\partial \mu_{r',t'}}{\partial m_{r,t}} \\ &= \frac{\partial \Phi(\mu)}{\partial m_{r,t}} = \frac{1}{5}. \end{aligned} \tag{5.18}$$

This allows us to compute

$$\begin{aligned} \frac{\partial \ln \tilde{G}(m)}{\partial m_{r,t}} &= \frac{1}{2} \ln m_{r,t} + \frac{1}{2} - \ln \mu_{r,t} - \sum_{r',t'} m_{r',t'} \frac{\partial \ln \mu_{r',t'}}{\partial m_{r,t}} \\ &= \frac{1}{2} \ln m_{r,t} - \ln \mu_{r,t} + \frac{3}{10}, \end{aligned} \tag{5.19}$$

and obtain the equations

$$\frac{1}{2} \ln m_{r,t} - \ln \mu_{r,t} + \frac{3}{10} = \lambda, \quad \forall r, t \in \{-1, 1\}, \tag{5.20}$$

where λ is the Lagrange multiplier introduced by the single constraint. After exponentiating (5.20), and defining $\lambda' = \exp(\lambda - 3/10)$, we can write

$$\frac{\sqrt{m_{r,t}}}{\mu_{r,t}} = \lambda', \quad \forall r, t \in \{-1, 1\}. \tag{5.21}$$

We relabel the entries of the matrices m and μ as

$$\begin{bmatrix} m_1 & m_2 \\ m_3 & m_4 \end{bmatrix}, \qquad \begin{bmatrix} \mu_1 & \mu_2 \\ \mu_3 & \mu_4 \end{bmatrix}.$$

Combining (5.21) and (5.8) and after some manipulations, we get

$$\mu_i \frac{\partial \Phi}{\partial \mu_j} - \mu_j \frac{\partial \Phi}{\partial \mu_i} = 0, \quad \forall i, j \in \{1, \ldots, 4\}.$$

We can factorize the following equation:

$$\mu_1 \frac{\partial \Phi}{\partial \mu_4} - \mu_4 \frac{\partial \Phi}{\partial \mu_1} = 0,$$

and get

$$(\mu_1 - \mu_4)\, P = 0,$$

where

$$\begin{aligned} P = \quad & 120\,\mu_1\,\mu_2\,\mu_3\,\mu_4 + 20\,\mu_1{}^3\,\mu_2 + 20\,\mu_1{}^3\,\mu_3 + 25\,\mu_1{}^3\,\mu_4 + 30\,\mu_1{}^2\,\mu_2{}^2 \\ & +30\,\mu_1{}^2\,\mu_3{}^2 + 35\,\mu_1{}^2\,\mu_4{}^2 + 5\,\mu_4{}^4 + 20\,\mu_1\,\mu_2{}^3 + 20\,\mu_1\,\mu_3{}^3 \\ & +25\,\mu_1\,\mu_4{}^3 + 5\,\mu_1{}^4 + 60\,\mu_1{}^2\,\mu_2\,\mu_3 + 80\,\mu_1{}^2\,\mu_2\,\mu_4 + 80\,\mu_1{}^2\,\mu_3\,\mu_4 \\ & +60\,\mu_2{}^2\,\mu_3\,\mu_4 + 60\,\mu_1\,\mu_2{}^2\,\mu_3 + 90\,\mu_1\,\mu_2{}^2\,\mu_4 + 60\,\mu_1\,\mu_2\,\mu_3{}^2 \\ & +80\,\mu_1\,\mu_2\,\mu_4{}^2 + 90\,\mu_1\,\mu_3{}^2\,\mu_4 + 80\,\mu_1\,\mu_3\,\mu_4{}^2 + 60\,\mu_2\,\mu_3{}^2\,\mu_4 \\ & +60\,\mu_2\,\mu_3\,\mu_4{}^2 + 20\,\mu_2{}^3\,\mu_3 + 20\,\mu_2{}^3\,\mu_4 + 30\,\mu_2{}^2\,\mu_3{}^2 + 30\,\mu_2{}^2\,\mu_4{}^2 \\ & +20\,\mu_2\,\mu_3{}^3 + 20\,\mu_2\,\mu_4{}^3 + 20\,\mu_3{}^3\,\mu_4 + 30\,\mu_3{}^2\,\mu_4{}^2 + 20\,\mu_3\,\mu_4{}^3, \end{aligned}$$

which is strictly positive, so $\mu_1 = \mu_4$. Similarly, we can factorize

$$\mu_2 \frac{\partial \Phi}{\partial \mu_3} - \mu_3 \frac{\partial \Phi}{\partial \mu_2} = 0,$$

and get

$$(\mu_2 - \mu_3)\, Q = 0,$$

where

$$\begin{aligned} Q = \quad & 120\,\mu_1\,\mu_2\,\mu_3\,\mu_4 + 20\,\mu_1{}^3\,\mu_2 + 20\,\mu_1{}^3\,\mu_3 + 20\,\mu_1{}^3\,\mu_4 + 30\,\mu_1{}^2\,\mu_2{}^2 \\ & +30\,\mu_1{}^2\,\mu_3{}^2 + 30\,\mu_1{}^2\,\mu_4{}^2 + 5\,\mu_3{}^4 + 5\,\mu_2{}^4 + 20\,\mu_1\,\mu_2{}^3 + 20\,\mu_1\,\mu_3{}^3 \\ & +20\,\mu_1\,\mu_4{}^3 + 90\,\mu_1{}^2\,\mu_2\,\mu_3 + 60\,\mu_1{}^2\,\mu_2\,\mu_4 + 60\,\mu_1{}^2\,\mu_3\,\mu_4 \\ & +80\,\mu_2{}^2\,\mu_3\,\mu_4 + 80\,\mu_1\,\mu_2{}^2\,\mu_3 + 60\,\mu_1\,\mu_2{}^2\,\mu_4 + 80\,\mu_1\,\mu_2\,\mu_3{}^2 \\ & +60\,\mu_1\,\mu_2\,\mu_4{}^2 + 60\,\mu_1\,\mu_3{}^2\,\mu_4 + 60\,\mu_1\,\mu_3\,\mu_4{}^2 + 80\,\mu_2\,\mu_3{}^2\,\mu_4 \\ & +90\,\mu_2\,\mu_3\,\mu_4{}^2 + 25\,\mu_2{}^3\,\mu_3 + 20\,\mu_2{}^3\,\mu_4 + 35\,\mu_2{}^2\,\mu_3{}^2 + 30\,\mu_2{}^2\,\mu_4{}^2 \\ & +25\,\mu_2\,\mu_3{}^3 + 20\,\mu_2\,\mu_4{}^3 + 20\,\mu_3{}^3\,\mu_4 + 30\,\mu_3{}^2\,\mu_4{}^2 + 20\,\mu_3\,\mu_4{}^3, \end{aligned}$$

which is also stricly positive, so $\mu_2 = \mu_3$. Finally, we substitute μ_4 by μ_1 and μ_3 by μ_2 in

$$\mu_1 \frac{\partial \Phi}{\partial \mu_2} - \mu_2 \frac{\partial \Phi}{\partial \mu_1} = 0,$$

and then factorize it to obtain

$$(\mu_1 - \mu_2)\, R = 0,$$

where

$$R = 70\, {\mu_1}^4 + 275\, {\mu_1}^3\, \mu_2 + 415\, {\mu_1}^2\, {\mu_2}^2 + 275\, \mu_1\, {\mu_2}^3 + 70\, {\mu_2}^4,$$

which is again strictly positive, so $\mu_1 = \mu_2$. Hence, all the μ_i are equal (and all the m_i are equal).

Since the m_i are equal and sum to 5/9, each must equal 5/36. Substituting this value into any of equations (5.8), and remembering that the μ_i are equal, gives each $\mu_i = 2^{-2/5}3^{-4/5}5^{-2/5}$. This shows that the Lagrange multiplier problem has a unique solution. This solution must correspond to the unique stationary point of $\tilde{G}$ in the interior of $\mathcal{M}'(1/9)$, which must then be a maximum.

Finally, (5.13) gives the maximizer of $\hat{G}$ in $\mathcal{D}'(1/9)$ when the $m_{r,t}$ (and the $\mu_{r,t}$) are fixed to be equal. The maximum value of $\hat{G}$ is computed from its definition. ∎

Now we recall the definition of the nine overlap variables from Section 4. We observe that (4.5) maps $\mathcal{D}$ into a polytope of dimension 4. The vectors $(n^{i,j})$ in this polytope can be expressed in terms of four variables by

$$\begin{aligned} &n^{0,2} = 1/3 - n^{0,0} - n^{0,1}, \quad n^{1,2} = 1/3 - n^{1,0} - n^{1,1}, \quad n^{2,0} = 1/3 - n^{0,0} - n^{1,0}, \\ &n^{2,1} = 1/3 - n^{0,1} - n^{1,1}, \quad n^{2,2} = n^{0,0} + n^{0,1} + n^{1,0} + n^{1,1} - 1/3, \end{aligned} \tag{5.22}$$

where the variables $n^{0,0}$, $n^{0,1}$, $n^{1,0}$ and $n^{1,0}$ take arbitrary nonnegative real values such that

$$n^{0,0}+n^{0,1} \le \frac{1}{3}, \quad n^{1,0}+n^{1,1} \le \frac{1}{3}, \quad n^{0,0}+n^{1,0} \le \frac{1}{3}, \quad n^{0,1}+n^{1,1} \le \frac{1}{3}, \quad n^{0,0}+n^{0,1}+n^{1,0}+n^{1,1} \ge \frac{1}{3}. \tag{5.23}$$

We are now in a good position to define the function F used in the statement of the Maximum Hypothesis. We first define the domain of F. This is the set of all nonnegative real vectors $\mathbf{n} = (n^{0,0}, n^{0,1}, n^{1,0}, n^{1,1})$ satisfying (5.23). For each $\mathbf{n}$ in the domain of F, we compute the nine overlap variables from (5.22) and define $F(\mathbf{n})$ to be the maximum of $\hat{F}(\mathbf{d})$ over $\mathcal{D}$ subject to the constraints in (4.5). This definition of F is repeated in Section 7, which also contains an alternative equivalent definition.

Let $\mathbf{b} = (b_s^{i,j})_{s\in\mathcal{S}, i,j\in\mathbb{Z}_3}$ be the point in $\mathcal{D}$ where $b_s^{i,j} = \frac{\binom{5}{s}}{8100}$ for all i, j, s. Now we return to our main function f, which was defined in (5.1).

Lemma 5.6 *Under the Maximum Hypothesis, the function f has a unique maximizer in $\mathcal{D}$ at $\mathbf{b}$. Moreover, $M := \max_{\mathbf{d}\in\mathcal{D}} \left\{5^{-5/2} e^{f(\mathbf{d})}\right\} = 25/24$.*

Proof. Recall that $f = \ln \hat{F}$. The Maximum Hypothesis implies that any maximizer of $\hat{F}$ on $\mathcal{D}$ must satisfy $\sum_{s\in\mathcal{S}} d_s^{i,j} = 1/9$, for all $i, j \in \mathbb{Z}_3$. Let us momentarily relax the constraints in (4.3), and maximize each factor

$$\hat{G}^{i,j}(\mathbf{d}) = \left(\prod_s \left(\frac{\binom{5}{s}}{d_s^{i,j}}\right)^{d_s^{i,j}}\right)\left(\prod_{r,t}(m_{r,t}^{i,j})^{\frac{1}{2}m_{r,t}^{i,j}}\right),$$

separately in $\mathcal{D}'(1/9)$. In view of Lemma 5.5, $\mathbf{b}$ is the unique maximizer and the maximum value of each factor is $(5^{5/2}25/24)^{1/9}$. We observe that the constraints in (4.3) are also satisfied by $\mathbf{b}$. Therefore $\mathbf{b}$ is the unique maximizer of $\hat{F}$ and the maximum function value is $\left((5^{5/2}25/24)^{1/9}\right)^9 = 5^{5/2}25/24$. ∎

5.2 Subexponential Factors

Here we complete the computation of the asymptotic expression of $\mathbf{E}(Y^2)$ under the Maximum Hypothesis by using a standard Laplace-type integration technique.

First we need the following result, whose proof we omit

Lemma 5.7 *The following system of* 24 *equations in the variables* $d_s^{i,j}$ *has rank* 23*:*

$$\sum_s s_1^t d_s^{i,j} - \sum_s s_{-1}^{-t} d_s^{i+1,j+t} = 0 \quad \forall i,j,t, \qquad \sum_{j,s} d_s^{i,j} = 1/3\ \forall i, \qquad \sum_{i,s} d_s^{i,j} = 1/3\ \forall j.$$

Moreover, after relabelling the variables as $d_1,\ldots,d_{324}$*, the solutions can be expressed by*

$$\begin{gathered} d_1,\ldots,d_{301} \quad \textit{free}, \\ d_k = L_k(d_1,\ldots,d_{301},1/6), \quad k=302,\ldots,324, \end{gathered}$$

where L_k *are linear functions with coefficients in* $\mathbb{Z}$*.*

Hereinafter, we relabel $d_s^{i,j}$ as $d_1,\ldots,d_{324}$ in the sense of Lemma 5.7. The $b_s^{i,j}$ are also relabelled as $b_1,\ldots,b_{324}$ accordingly. (Recall that $b_s^{i,j}$ was defined as $\binom{5}{s}/8100$.) For a point $\mathbf{d} = (d_1,\ldots,d_{324}) \in \mathcal{D}$, the first 301 coordinates will be often denoted by $\tilde{\mathbf{d}} = (d_1,\ldots,d_{301})$ for simplicity.

Let $\epsilon > 0$ be fixed but small enough. We consider the cube of side 2ϵ centered on $\tilde{\mathbf{b}}$

$$\tilde{\mathcal{Q}} = \{(d_1,\ldots,d_{301}) \in \mathbb{R}^{301} \ : \ d_k \in [b_k-\epsilon, b_k+\epsilon],\ \forall k\}$$

and the discrete subset

$$\tilde{\mathcal{J}} = \tilde{\mathcal{Q}} \cap \left(\frac{1}{n}\mathbb{Z}^{301}\right).$$

Let us define their extension to higher dimensions:

$$\begin{aligned} \mathcal{Q} = \{ \quad & (d_1,\ldots,d_{324}) \in \mathbb{R}^{324} \ : \ (d_1,\ldots,d_{301}) \in \tilde{\mathcal{Q}}, \\ & d_k = L_k(d_1,\ldots,d_{301},1/6),\ \forall k = 302,\ldots,324\}, \end{aligned}$$

where the L_k's are as in Lemma 5.7, and

$$\mathcal{J} = \mathcal{Q} \cap \left(\frac{1}{n} \mathbb{Z}^{324} \right).$$

Note that $\mathbf{b}$ is an interior point of $\mathcal{D}$, and that for each k the function $L_k(\cdot, 1/6)$ is continuous. Then, if ϵ is chosen small enough, we can ensure that for some $\delta > 0$

$$\forall \mathbf{d} \in \mathcal{Q}, \quad d_k > \delta \text{ and } |d_k - b_k| < \delta, \quad k = 1, \ldots, 324, \tag{5.24}$$

and hence $\mathcal{Q} \subset \mathcal{D}$. Moreover, since n is always divisible by 6, for each k the function $L_k(\cdot, 1/6)$ maps points from $\frac{1}{n}\mathbb{Z}^{301}$ into $\frac{1}{n}\mathbb{Z}$, and so $\mathcal{J} \subset \mathcal{I}$.

Now recalling the definitions of f, g and h in (5.1), we define for any $(d_1, \ldots, d_{301}) \in \tilde{\mathcal{Q}}$

$$\begin{array}{l} \tilde{f}(d_1, \ldots, d_{301}) = f(d_1, \ldots, d_{324}) \\ \tilde{g}(d_1, \ldots, d_{301}) = g(d_1, \ldots, d_{324}) \end{array}, \quad \text{where } d_k = L_k(d_1, \ldots, d_{301}, 1/6), \ \forall k = 302, \ldots, 324.$$

From Lemma 5.6 and by straightforward computations we obtain the following:

Lemma 5.8 *The following statements hold:*

- *Under the Maximum Hypothesis, f has a unique maximum in $\mathcal{D}$ at $\mathbf{b}$.*
- *Under the Maximum Hypothesis, $\tilde{f}$ has a unique maximum in $\tilde{\mathcal{Q}}$ at $\tilde{\mathbf{b}}$, with $e^{f(\mathbf{b})} = e^{\tilde{f}(\tilde{b})} = \frac{25}{24} 5^{5/2} \approx 58.2309$.*
- *The Hessian $\tilde{H}$ of $\tilde{f}$ at $\tilde{\mathbf{b}}$ is negative definite, and* $\det \tilde{H} = -2^{175} 3^{1078} 5^{310} 7^{12} 11^{14} 13 \cdot 17 \ 79^4$.
- $\tilde{g}(\tilde{\mathbf{b}}) = 2^{90} 3^{558} 5^{171} \neq 0$.
- *Both $\tilde{f}$ and $\tilde{g}$ are of class C^∞ in $\tilde{\mathcal{Q}}$.*

We compute the contribution to $\mathbf{E}(Y^2)$ of the terms around $\mathbf{b}$ and get the following.

Lemma 5.9 *Under the Maximum Hypothesis,*

$$\sum_{\mathbf{d} \in \mathcal{J}} q(n, \mathbf{d}) e^{f(\mathbf{d})n} \sim \frac{(2\pi n)^{301/2}}{\sqrt{|\det \tilde{H}|}} \tilde{g}(\tilde{\mathbf{b}}) e^{n\tilde{f}(\tilde{\mathbf{b}})} = \frac{2^3 3^{19} 5^{16} (2\pi n)^{301/2}}{7^6 11^7 79^2 \sqrt{2 \ 13 \cdot 17}} \left(\frac{25}{24} \right)^n 5^{5n/2}.$$

Proof. From (5.24), we see that for all $\mathbf{d} \in \mathcal{J} \subset \mathcal{Q}$ we must have $d_k > \delta \ \forall k$. Thus, by their definition, all the $m_{r,t}^{i,j}$ are bounded away from 0, $q(n, \mathbf{d}) \sim g(\mathbf{d})$ and we can write

$$\sum_{\mathbf{d} \in \mathcal{J}} q(n, \mathbf{d}) e^{f(\mathbf{d})n} \sim \sum_{\mathcal{J}} g(\mathbf{d}) e^{nf(\mathbf{d})} = \sum_{\tilde{\mathcal{J}}} \tilde{g}(\tilde{\mathbf{d}}) e^{n\tilde{f}(\tilde{\mathbf{d}})}. \tag{5.25}$$

We note that both $\tilde{f}$ and $\tilde{g}$ and its partial derivatives up to any fixed order are uniformly bounded in the compact set $\tilde{\mathcal{Q}}$. Then, by repeated application of the Euler-Maclaurin summation formula (see [1], p. 806), we have asymptotically as n grows large

$$\sum_{\tilde{\mathcal{J}}} \tilde{g}(\tilde{\mathbf{d}}) e^{n\tilde{f}(\tilde{\mathbf{d}})} \sim n^{301} \int_{\tilde{\mathcal{Q}}} \tilde{g}(\tilde{x}) e^{n\tilde{f}(\tilde{x})} d\tilde{x}. \tag{5.26}$$

We observe from Lemma 5.8 that we are in good condition to apply Laplace's method as developed in the multivariate case by Wong [16, Theorem IX.5.3]. We obtain

$$\int_{\tilde{\mathcal{Q}}} \tilde{g}(\tilde{x}) e^{n\tilde{f}(\tilde{x})} d\tilde{x} \sim \frac{1}{\sqrt{|\det \tilde{H}|}} \left(\frac{2\pi}{n}\right)^{301/2} \tilde{g}(\tilde{\mathbf{b}}) e^{n\tilde{f}(\tilde{\mathbf{b}})}. \tag{5.27}$$

The result follows from (5.25), (5.26), (5.27) and Lemma 5.8. ∎

Now we deal with the remaining terms of the sum.

Lemma 5.10 *Under the Maximum Hypothesis, there exists some positive real $\alpha < e^{f(\mathbf{b})}$ s.t.* $\sum_{\mathcal{I}\setminus\mathcal{J}} q(n, \mathbf{d}) e^{f(\mathbf{d})n} = o(\alpha^n)$.

Proof.

Let B be the topological closure of $\mathcal{D}\setminus\mathcal{Q}$. We recall from Lemma 5.8 that f has a unique maximum in $\mathcal{D}$ at point $\mathbf{b} \notin B$. Then, since B is a compact set and f is continuous, there must be some real $\beta < f(\mathbf{b})$ such that $f(\bar{x}) \leq \beta \ \forall \bar{x} \in B$. Now we observe that all terms in the sum $\sum_{\mathcal{I}\setminus\mathcal{J}} q(n, \mathbf{d}) e^{f(\mathbf{d})n}$ can be uniformly bounded by $Cn^{162}e^{\beta n}$, for some fixed constant C. Note furthermore that there is a polynomial number of terms (at most $(n+1)^{324}$) in the sum. Hence, the result holds by taking for instance $\alpha = (e^{\beta} + e^{f(\mathbf{b})})/2$. ∎

From Lemmata 5.9 and 5.10,

$$\sum_{\mathcal{I}} g(\mathbf{d}) e^{f(\mathbf{d})n} \sim \frac{2^3 3^{19} 5^{16} (2\pi n)^{301/2}}{7^6 11^7 79^2 \sqrt{2\ 13 \cdot 17}} \left(\frac{25}{24}\right)^n 5^{5n/2}$$

and finally, from this and Lemma 5.1, we conclude the following.

Theorem 5.1 *Under the maximum hypothesis,*

$$\mathbf{E}(Y^2) \sim \frac{2^2 3^{19} 5^{16}}{7^6 11^7 79^2 \sqrt{13 \cdot 17}} \frac{1}{(2\pi n)^2} \left(\frac{25}{24}\right)^n,$$

which is (2.5).

6 ...and for n not divisible by 6

Since 5-regular graphs have an even number of vertices, we only need to consider $n \equiv 2$ or 4 (mod 6).

One possibility is to rework the whole argument of this paper but with slightly unbalanced colourings. Instead, the asymmetry in the argument can be somewhat reduced by using an argument relating different models of random regular graphs. We first treat the case $n \equiv 0$ (mod 6) in more depth, and prove the following.

Theorem 6.1 *Fix nonnegative integers j^*_{12}, j^*_{23} and j^*_{13} and set $j^* = j^*_{12} + j^*_{23} + j^*_{13}$. Consider the 5-regular graphs with $n \equiv 0$ (mod 6) vertices and a distinguished ordered set of j^* edges, no two being incident with the same vertex. Let G be chosen uniformly at random from such structures. Under the Maximum Hypothesis, G a.a.s. has a 3-colouring in which the first j^*_{12} distinguished edges have end vertices coloured 1 and 2, the next j^*_{23} have end vertices coloured 2 and 3, and the rest have end vertices coloured 1 and 3.*

Proof. Consider the probability space Ω_n with uniform probability distribution, and whose underlying set consists of pairings in $\mathcal{P}_{n,5}$ with an ordered set J of j^* distinguished pairs of points, such that no two pairs in J are incident with the same vertex. Let $\hat{Y}$ denote the number of locally rainbow balanced 3-colourings of a pairing containing J, in which the distinguished pairs join vertices of the preassigned colours. We will show that

$$\mathbf{E}\hat{Y} \sim 3^{-j^*}\mathbf{E}Y, \tag{6.1}$$

that (3.2) holds with Y replaced by $\hat{Y}$ (and no other adjustment), and that under the Maximum Hypothesis,

$$\mathbf{E}(\hat{Y}^2) \sim 9^{-j^*}\mathbf{E}(Y^2). \tag{6.2}$$

The theorem then follows immediately by the argument in the last few sentences of the proof of Theorem 1.1.

To show (6.1), we apply the same method as in the proof of Theorem 1.1. First, rework the proof of Lemma 3.1, but after assigning vertices to colour classes, select which pairs are in J. This can be done in asymptotically $(5n/3)^{2j^*}$ ways, since each distinguished pair must join points belonging to vertices of two given colour classes, and if such pairs of vertices are randomly chosen, a.a.s. no vertex is repeated. Then, for those vertices containing a point in a pair in J, the generating function $(x+1)^5 - x^5 - 1$ is adjusted to either $(x+1)^4 - x^4$ or $(x+1)^4 - 1$ since the choice of colour for the mate of one of the points is already determined. (Compare this with the similar adjustments made in the derivation of (3.2).) Finally, the (remaining parts of the) matchings between colour classes are chosen as before, so between two colour classes where there are j_0 distinguished edges, the number of matchings is $(5n/6 - j_0)!$. On the other hand, the total number of choices of the pairing with the ordered set J distinguished is asymptotically $(5n/2)^{j^*}|\mathcal{P}_{n,d}|$, since we can choose first the pairing and next the distinguished edges at random. These will satisfy the nonadjacency condition a.a.s.

Comparing with the computation of $\mathbf{E}Y$, this produces

$$\mathbf{E}\hat{Y} \sim \frac{(5n/3)^{2j^*}15^{2j^*}}{30^{2j^*}(5n/6)^{j^*}(5n/2)^{j^*}}\mathbf{E}Y = 3^{-j^*}\mathbf{E}Y,$$

as required for (6.1).

To verify (3.2) with $\hat{Y}$ in place of Y, we note that the calculation of $\mathbf{E}(\hat{Y}X_k)$ requires the same modifications as $\mathbf{E}\hat{Y}$. In particular, the same adjustment of factors in the generating functions is warranted. So $\mathbf{E}(\widehat{YX_k}) \sim 3^{-j^*}\mathbf{E}\hat{Y}$. The same argument shows that

$$\mathbf{E}(\hat{Y}[X_1]_{m_1}\cdots[X_j]_{m_j}) \sim 3^{-j^*}\mathbf{E}(Y[X_1]_{m_1}\cdots[X_j]_{m_j})$$

and thus (3.2) holds with Y replaced by $\hat{Y}$. As before, δ_k is defined by (3.1).

To estimate $\mathbf{E}(\hat{Y}^2)$, there is no need to adjust the formulae in Section 4, though that would be one way to achieve the result. Instead, note that, corresponding to (4.1),

$$\mathbf{E}(\hat{Y}^2) = \frac{|\{(P,C_1,C_2,J) \mid P \in \mathcal{P}_{n,5}, J \in \mathcal{J}_P, C_1, C_2 \in \mathcal{R}_{P,J}\}|}{|\{(P,J) \mid P \in \mathcal{P}_{n,5}, J \in \mathcal{J}_P\}|},$$

where $\mathcal{J}_P$ denotes the set of ordered j^*-subsets of pairs of P that do not contain common vertices, and $\mathcal{R}_{P,J}$ denotes the set of locally rainbow balanced 3-colourings of P that give the required colours to the ends of edges in J. Since almost all choices of j^* pairs do not intersect at vertices, we have

$$\frac{|\{(P,J) \mid P \in \mathcal{P}_{n,5}, J \in \mathcal{J}_P\}|}{|\mathcal{P}_{n,5}|} \sim \left(\frac{5n}{2}\right)^{j^*}.$$

On the other hand, we show below that

$$\frac{|\{(P,C_1,C_2,J) \mid P \in \mathcal{P}_{n,5}, J \in \mathcal{J}_P, C_1, C_2 \in \mathcal{R}_{P,J}\}|}{|\{(P,C_1,C_2) \mid P \in \mathcal{P}_{n,5}, C_1, C_2 \in \mathcal{R}_P\}|} \sim \left(\frac{5n}{18}\right)^{j^*}. \tag{6.3}$$

Comparing with (4.1) then gives (6.2).

To complete the proof of the theorem, it is only required to show (6.3). We may rewrite the numerator on its left side as

$$\sum_{|\{(P,C_1,C_2) \mid P \in \mathcal{P}_{n,5}, C_1, C_2 \in \mathcal{R}_P\}|} h(P,C_1,C_2) \tag{6.4}$$

where h gives the number of choices of the ordered set J of j^* pairs that have the required colours at their ends in both colourings C_1 and C_2. It is easy to see, from Lemmata 5.1 and 5.6, that under the maximum hypothesis, the contribution to $\mathbf{E}(Y^2)$ from $\mathbf{d}$ where $d_s^{i,j} \sim b_s^{i,j}$ is $\mathbf{E}(Y^2)(1+o(1))$. For such points of the domain, all $m_{r,t}^{i,j}$ are asymptotically equal to $5/36$ and all $n^{i,j}$ are asymptotically equal to $1/9$. Thus, considering how (4.1) led to Lemma 5.1, almost all of the triples (P,C_1,C_2) being summed over in (6.4) have asymptotically $5n/36$ edges between any two parts $V^{i,j}$ and $V^{i',j'}$ in the partition of vertices generated by C_1 and C_2. For these triples, $h(P,C_1,C_2)$ is asymptotic to $(5n/18)^{j^*}$, since two adjacent vertices of the same two colours in both C_1 and C_2 can have either the same colour or opposite colours in the two colourings. On the other hand, it is immediate that

$$h(P,C_1,C_2) = O(n^{j^*})$$

and hence the contribution to (6.4) from the other $\mathbf{d}$ is negligible. Thus the expression in (6.4) is asymptotic to

$$\left(\frac{5n}{18}\right)^{j^*} |\{(P, C_1, C_2) \mid P \in \mathcal{P}_{n,5}, C_1, C_2 \in \mathcal{R}_P\}|.$$

and (6.3) follows. ∎

Proof of Theorem 1.1 (for n not divisible by 6) We use the type of argument employed at the end of Section 3 of [13]. Suppose $n \equiv 2 \pmod 6$. Take a random 5-regular graph G with n vertices, and assume without loss of generality (by relabelling vertices say) that the last two vertices, call them u and v, are adjacent in G. Delete u and v, and join up the former neighbours of u using two new edges, and the same with the former neighbours of v, in each case randomly choosing how to pair up the four neighbours. Leave the four added edges as a distinguished ordered set of edges, the first two joining former neighbours of u and the last two similarly for v. It is easy to show and well known that a given vertex of a random 5-regular graph is a.a.s. not in a cycle of length less than 4 (or 100, for that matter). It follows that a.a.s. no multiple edges occur due to the new edges, and furthermore that a.a.s. the new edges are not adjacent to each other. Throw the graph away if either of these two properties fails to hold. The result is a random 5-regular graph with an ordered set of distinguished edges, no two adjacent. Let us call this G'.

The distribution of G' is not uniform, as it is for the random structures in Theorem 6.1. The probability that G' occurs is proportional to the number of ways of reinstating the edges to u and v. This is the same for all graphs in which there are no edges joining any vertices incident with the distinguished edges. Almost all choices of a set of distinguished edges in a regular graph will have this property, and so it follows that any property a.a.s. true for the random structures in Theorem 6.1 with $j^* = 4$ is a.a.s. true for G'.

Thus, by Theorem 6.1, G' a.a.s. has a 3-colouring such that the first two distinguished edges join vertices of colours 1 and 2, and the others join vertices of colours 1 and 3. Then by we can use exactly this colouring on $V(G) \setminus \{u, v\}$, and colour u with colour 2 and v with colour 1, to obtain a 3-colouring of G.

For $n \equiv 4 \pmod 6$, we may apply exactly the same argument, but deleting two pairs of adjacent vertices rather than one pair. ∎

7 The Maximum Hypothesis and its Empirical Validation

In this section we describe the evidence which supports the Maximum Hypothesis. The hypothesis asserts that for a certain four-variable function $F(\mathbf{n})$ on a bounded domain, $F(\mathbf{n})$ has a unique global maximum at the point $(1/9, 1/9, 1/9, 1/9)$. There are two equivalent definitions for the function F, which give two possible approaches to numerical verification of the Maximum Hypothesis. All the relevant definitions and equations are repeated here, so that the definition of F in this section is self-contained.

We first define the domain of F. This is the set of all nonnegative real vectors $\mathbf{n} = (n_1, \dots, n_4)$ satisfying

$$n_1 + n_2 \le \frac{1}{3}, \quad n_3 + n_4 \le \frac{1}{3}, \quad n_1 + n_3 \le \frac{1}{3}, \quad n_2 + n_4 \le \frac{1}{3}, \quad n_1 + n_2 + n_3 + n_4 \ge \frac{1}{3}. \tag{7.1}$$

For each $\mathbf{n}$ in the domain of F, we define the following nine values

$$\begin{array}{lll} n^{0,0} = n_1, & n^{0,1} = n_2, & n^{0,2} = 1/3 - n_1 - n_2 \\ n^{1,0} = n_3, & n^{1,1} = n_4, & n^{1,2} = 1/3 - n_3 - n_4 \\ n^{2,0} = 1/3 - n_1 - n_3, & n^{2,1} = 1/3 - n_2 - n_4, & n^{2,2} = n_1 + n_2 + n_3 + n_4 - 1/3 \end{array} \tag{7.2}$$

We need some more definitions before stating how to compute F at any point in its domain.

A *spectrum* s is a 2×2 nonnegative integer matrix such that each row and column sum is at least 1, and the sum of all four entries is 5. We index the rows and columns by -1 and 1, with -1 for the first row or column. So

$$s = \begin{bmatrix} s_{-1,-1} & s_{-1,1} \\ s_{1,-1} & s_{1,1} \end{bmatrix}.$$

Let $\mathcal{S}$ denote the set of all spectra, including $\begin{bmatrix} 4 & 0 \\ 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 3 & 0 \\ 1 & 1 \end{bmatrix}$ and so on. Note that $|\mathcal{S}| = 36$. (This definition of spectrum is the same as the one presented in Section 4).

For each ordered pair (i, j), $i, j \in \mathbb{Z}_3$, and spectrum $s \in \mathcal{S}$, introduce a real variable $d_s^{i,j}$, called a *spectral* variable. Also define matrices $m^{i,j}$ by

$$m^{i,j} = \sum_{s \in \mathcal{S}} d_s^{i,j}\, s. \tag{7.3}$$

(cf. (4.4))

Consider the following as constraints for all i and j:

$$\sum_{s \in \mathcal{S}} d_s^{i,j} = n^{i,j}, \quad d_s^{i,j} \ge 0 \ \forall s \in \mathcal{S}, \tag{7.4}$$

where the constants $n^{i,j}$ are defined in (7.2), and

$$m_{r,t}^{i,j} = m_{-r,-t}^{i+r,j+t}, \quad \text{for } i, j \in \{0,1,2\} \ \text{ and } r, t \in \{-1, 1\}, \tag{7.5}$$

where the arithmetic in the indices is modulo 3.

For a sequence $\mathbf{d}$ of variables $d_s^{i,j}$ satisfying the above constraints, let $\hat{F}(\mathbf{d})$ be the function defined as

$$\hat{F}(\mathbf{d}) = \left(\prod_{i,j,s} \left(\frac{\binom{5}{s}}{d_s^{i,j}} \right)^{d_s^{i,j}} \right) \left(\prod_{i,j,r,t} (m_{r,t}^{i,j})^{\frac{1}{2} m_{r,t}^{i,j}} \right). \tag{7.6}$$

(We follow the convention that 0^0 equals 1.) Note that $\hat{F}$ is a function of 9×36 constrained variables. Since $\hat{F}$ is continuous in the compact domain defined by the constraints, it must have a maximum. Then, we set $F(\mathbf{n})$ to be the value of this maximum.

In Section 5 we defined the same function $\hat{F}(\mathbf{d})$ but extended it to the larger domain $\mathcal{D}$ where the $n^{i,j}$ are not fixed but rather take any value in (7.2).

For the second definition of F, define the matrix function (also defined as (5.7))

$$\Phi \begin{bmatrix} x & y \\ z & w \end{bmatrix} = (x+y+z+w)^5-(x+y)^5-(x+z)^5-(y+w)^5-(z+w)^5+x^5+y^5+z^5+w^5. \quad (7.7)$$

For each of the nine possible pairs (i,j), $i,j \in \mathbb{Z}_3$, let $\mu^{i,j}$ and $m^{i,j}$ be 2×2 matrices whose rows and columns are indexed by -1 and 1 (as in the first definition of F). For each such (i,j), consider the 4×4 system (cf. (5.8))

$$\frac{\partial\ \Phi\mu^{i,j}}{\partial \mu^{i,j}_{r,t}}\ \mu^{i,j}_{r,t} = m^{i,j}_{r,t}, \quad r,t = -1, 1. \quad (7.8)$$

As in (5.4), we consider the following constraints, for all such i and j, and all $r,t \in \{-1,1\}$,

$$\begin{array}{rcl} m^{i,j}_{r,t} & \geq & 0, \\ m^{i,j}_{r,t} + m^{i,j}_{r,-t} & \leq & 4(m^{i,j}_{-r,t} + m^{i,j}_{-r,-t}), \\ m^{i,j}_{r,t} + m^{i,j}_{-r,t} & \leq & 4(m^{i,j}_{r,-t} + m^{i,j}_{-r,-t}). \end{array} \quad (7.9)$$

For each $\mathbf{n}$ in the domain of F, we define $\mathcal{M}(\mathbf{n})$ to be the set of all vectors $\mathbf{m} = (m^{i,j})_{i,j\in\mathbb{Z}_3}$ of 2×2 matrices $m^{i,j}$ satisfying (7.9), (7.5), and also

$$\sum_{r,t} m^{i,j}_{r,t} = 5n^{i,j}, \quad (7.10)$$

where the constants $n^{i,j}$ are defined in (7.2). We observe that $\mathcal{M}(\mathbf{n})$ is a polytope of dimension 9. Given a vector $\mathbf{m}$ of matrices $(m^{i,j})_{i,j\in\mathbb{Z}_3}$ in the interior of $\mathcal{M}(\mathbf{n})$, define

$$\tilde{F}(\mathbf{m}) = \prod_{i,j,r,t} \left(\frac{(m^{i,j}_{r,t})^{\frac{1}{2}}}{\mu^{i,j}_{r,t}} \right)^{m^{i,j}_{r,t}}, \quad (7.11)$$

with the $\mu^{i,j}_{r,t}$ given in terms of the $m^{i,j}_{r,t}$ by (7.8) and required to be strictly positive. In Section 5, we show that for $\mathbf{m}$ in the interior of $\mathcal{M}(\mathbf{n})$ the $\mu^{i,j}_{r,t}$ variables are determined uniquely, and that $\tilde{F}$ can be continuously extended to the boundary points of the polytope.

Our second definition of $F(\mathbf{n})$ is the maximum of $\tilde{F}(\mathbf{m})$ over all $\mathbf{m}$ lying in $\mathcal{M}(\mathbf{n})$. This is well defined by continuity of the function and compactness of the domain.

We observe that Lemma 5.3 shows the equivalence of these two alternative definitions of F.

One important piece of evidence supporting the Maximum Hypothesis is the following theorem.

Theorem 7.1 *The function $F(\mathbf{n})$ has a local maximum at the point* $(1/9, 1/9, 1/9, 1/9)$.

Proof. By Lemma 5.5, $\hat{G}(\mathbf{d})$ takes its maximum in $D'(1/9)$ uniquely at the point where all the d_s are equal to $\binom{5}{s}/8100$. It follows by continuity of $\hat{F}$ that the only values of $\hat{F}$ that can contribute to the maximum value of F in a neighbourhood of $(1/9, 1/9, 1/9, 1/9)$ must come from $\mathbf{d}$ in a neighbourhood of $(\binom{5}{s}/8100)_{s\in\mathcal{S}}$. The Hessian, computed using Maple, shows that $\hat{F}$ has a local maximum here, so the local maximum of F at $(1/9, 1/9, 1/9, 1/9)$ follows. ∎

Next, we describe the empirical evidence that F has a unique maximum at $(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9})$.

Let $\mathbf{n}$ be any fixed vector in the domain of F. Recall the definition of $\mathcal{M}'(c)$ from Section 5.1. We observe that the projection of $\mathcal{M}(\mathbf{n})$ to the (i, j) coordinate is $\mathcal{M}'(n^{i,j})$. Let us momentarily relax the constraints in (7.5), and consider separately each factor

$$\tilde{G}^{i,j} = \prod_{r,t} \left(\frac{(m^{i,j}_{r,t})^{\frac{1}{2}}}{\mu^{i,j}_{r,t}} \right)^{m^{i,j}_{r,t}}$$

to be defined in $\mathcal{M}'(n^{i,j})$. We note that $\mathcal{M}'(n^{i,j})$ is a polytope of dimension 3, so $G^{i,j}$ can be written in terms of three free variables. In order to show that $\ln \tilde{G}^{i,j}$ is concave, it is sufficent to see that the 3×3 Hessian matrix is negative definite over the domain. This was numerically confirmed with the help of a computer. Having experimentally confirmed the concavity of the logarithm of each factor of $\tilde{F}$, we conclude the concavity of $\ln \tilde{F}$. Moreover, this concavity is not affected by adding the constraints in (7.5), previously relaxed.

The procedure we use is based on the concavity of $\ln \tilde{F}$. We sweep the domain of F. Variables n_1, n_2, n_3, n_4 take all nonnegative values satisfying (7.1) in a grid of 200 steps per dimension. For each point $\mathbf{n} = (n_1, \ldots, n_4)$ we compute $F(\mathbf{n})$ as follows.

Procedure for computing $F(\mathbf{n})$.

1. We compute the nine overlap variables $n^{i,j}$ from (7.2). (The sweep avoids a fine layer of width 1/1000 around the boundary.)

2. We set $\mathbf{m}_0$ to be an interior point of $\mathcal{M}(\mathbf{n})$.

3. Starting from $\mathbf{m}_0$, we numerically maximize $\ln \tilde{F}$ in $\mathcal{M}(\mathbf{n})$ by some Newton-like iterative method. This should work reasonably well from the concavity of $\ln \tilde{F}$. As we observed before, the maximization domain has dimension 9. In fact, the elements in $\mathcal{M}(\mathbf{n})$ can be expressed in terms of the nine coordinates $m^{i,j}_{1,1}$ by

$$\begin{aligned}
m^{i,j}_{-1,-1} &= m^{i-1,j-1}_{1,1} \\
m^{i,j}_{1,-1} &= \tfrac{1}{2}\left(a^{i,j} + a^{i+1,j-1} - a^{i-1,j+1}\right) \\
m^{i,j}_{-1,1} &= \tfrac{1}{2}\left(a^{i,j} + a^{i-1,j+1} - a^{i+1,j-1}\right),
\end{aligned}$$

where

$$a^{i,j} = 5n^{i,j} - m^{i,j}_{1,1} - m^{i-1,j-1}_{-1,-1}.$$

Then we must write $\ln \tilde{F}$ in terms of the $m^{i,j}_{1,1}$ and, at each step of the maximization, compute the gradient with respect to these nine variables. From the proof of Lemma 5.5 and in view of (5.19), we can get rid of the derivatives of the $\mu^{i,j}_{r,t}$ and express this gradient just in terms of the $m_{r,t}^{i,j}$ and $\mu_{r,t}^{i,j}$. Hence, each iteration of the maximization algorithm requires the solution of the nine 4×4 sytems in (7.8), which are known to have a unique positive solution.

The maximum obtained is $F(\mathbf{n})$.

Recall from Lemma 5.6 that $F(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9}) = 5^{5/2}25/24 \approx 58.2309$. The values of F we obtained by this procedure for each $\mathbf{n}$ were always below $F(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9})$. There were some points in the domain where a value over 58 was obtained. These points were all near $(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9})$. Around these points we made an additional scan of the neighbourhood with stepsize 1/8000. The values obtained were always less than $F(\frac{1}{9}, \frac{1}{9}, \frac{1}{9}, \frac{1}{9})$.

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