

TREE AND FOREST WEIGHTS AND THEIR APPLICATION TO NONUNIFORM RANDOM GRAPHS

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For a complete graph K_n on n vertices with weighted edges, define the weight of a spanning tree (more generally, spanning forest) as the product of edge weights involved. Define the tree weight (forest weight) of K_n as the total weight of all spanning trees (forests). The uniform edge weight distribution is shown to maximize the tree weight, and an explicit bound on the tree weight is formulated in terms of the overall variance of edge weights as well as the variance of the sum of edge weights over nodes. An application to sparse random graphs leads to a bound for the relative risk of observing a spanning tree in a well-defined neighborhood of the uniform distribution. An analogous result shows that, for each positive integer k , the weight of all forests with k rooted trees is also maximized under the uniform distribution. A key ingredient for the latter result is a formula for the weight of forests of k rooted trees that generalizes Maxwell's rule for spanning trees. Our formulas also enable us to show that the number of trees in a random rooted forest is intrinsically divisible, that is, representable as a sum of n independent binary random variables ε_j , with parameter $(1 + \lambda_j)^{-1}$, λ_j 's being the eigenvalues of the Kirchhoff matrix. This is directly analogous to the properties of the number of blocks in a random set partition (Harper), of the size of the random matching set (Godsil) and of the number of leaves in a random tree (Steele).

1. Introduction. Various classes \mathcal{C} of objects, such as permutations, groups, trees and directed graphs have natural representations in terms of matrices. Several authors [e.g., Beran (1979), Verducci (1989)] have investigated probability models on these classes in terms of exponential families based on such matrix representations. That is, if $R(\pi)$ is a square matrix representing object π and Θ is a parameter matrix of the same dimensions, then

$$(1) \quad P(\pi) = \frac{\exp\{\text{tr}[R(\pi)' \Theta]\}}{\psi(\Theta)}$$

is the probability density (with respect to Haar measure for continuous groups or counting measure for finite classes) of the associated family.

An area of interest is the form of the normalizing constant

$$(2) \quad \psi(\Theta) = \sum_{\pi \in \mathcal{C}} \exp\{\text{tr}[R(\pi)' \Theta]\}.$$

For example, when \mathcal{C} is the symmetric group S_n of all permutations π of $[n] \equiv \{1, \dots, n\}$ and $R(\pi)$ is the corresponding permutation matrix, then

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$\psi(\Theta)$ is the *permanent* of $A \equiv [\exp(\Theta_{ij})]$; that is,

$$\psi_{S_n}(\Theta) = \sum_{\pi \in S_n} \prod_{i=1}^n A_{i\pi(i)}$$

[see Minc (1978) for a thorough treatment of permanents]. The recently proved van der Waerden conjecture [see van Lint and Wilson (1992), Chapter 12] asserts that ψ is *minimized* over all doubly stochastic matrices A when all the entries of A are equal (i.e., $A = [1/n]$.) Extrema of $\psi_{\mathcal{C}}$ for other classes \mathcal{C} is of central focus to this paper.

Of particular interest is the situation where \mathcal{C} consists of all n^{n-2} spanning trees π on $[n]$ (identified with the n vertices labelled $1, 2, \dots, n$), and the $n \times n$ symmetric matrix $R(\pi)$ has (i, j) and (j, i) entries 1 if the tree π has edge $e = (i, j)$, [that is, if $e \in E(\pi)$, the set of all edges in the tree π], and 0 otherwise. In this case, we can simplify notation by treating A as a symmetric matrix (e.g., an adjacency matrix with entries indicating edge weights). Then the $n \times n$ matrix A may be identified with its edge weights $\{a_e, e \in E(K_n)\}$, and

$$\begin{aligned} \psi_{\text{tree}}(\Theta) &= \sum_{\pi \in \mathcal{C}} \prod_{e \in E(\pi)} a_e \\ (3) \qquad \qquad &\equiv t(A) \end{aligned}$$

is called the *tree weight* of A . The tree weight $t(A)$ is also called the *tree polynomial* [Farrell (1981)] of the complete graph K_n on n nodes with weighted edges because it is a polynomial in the entries a_e of A and the summation is over all n^{n-2} spanning trees of K_n . Individual terms in (3) are called *tree products*.

When A is the adjacency matrix of a simple graph G , then $t(A)$ clearly counts the number of spanning trees of G . In this paper, the tree weight $t(A)$ naturally arises with more general forms of A . For $A = [o_e]$ assigning odds o_e to all edges e of K_n , $t(A)$ becomes the key to calculating the probability of observing a spanning tree on n nodes when edges $e \in K_n$, appear independently with probabilities $p_e = o_e/(1 + o_e)$. Also, if $p_e = c_e/n$ (generating a “sparse” random graph), then the expected number of tree components having k nodes is easily shown to be asymptotically equal to a weighted sum of $t(A_S)$, where $S \subset [n]$, $|S| = k$ and $A_S = \{a_e: e \in S \times S\}$.

The authors conjectured [Jones (1995)] that, given the total edge weight $w = \sum_e a_e$, $t(A)$ attains its maximum at the uniform weight distribution $a_e^* = w/N$, where $N = \binom{n}{2}$ is the number of edges in the edge set $E(K_n)$. In Section 2 we prove this conjecture and also obtain an upper bound for the ratio $t(A)/t(A^*)$ expressed in terms of the first and second empirical moments of the vertex weights $a_i \equiv \sum_{e \ni i} a_e$.

We use these results in Section 3 to investigate a sparse random graph model. Specifically, we look at the probability that the random graph is a spanning tree, comparing it to the uniform case with $p_e = \bar{c}/n$, $\bar{c} = N^{-1} \sum_e c_e$. The limiting ratio of the corresponding probabilities is bounded from above

in terms of the first two empirical moments of the edge weights $[c_e]$ and the vertex weights $[c_i]$. The bound implies that, in a nondegenerate situation, the probability is maximum in the uniform case for n large, provided that the average edge weight \bar{c} strictly exceeds 4 in the limit. We conclude the section with a simple example indicating that this bound for \bar{c} cannot be pushed below $2 + \sqrt{2}$.

In Section 4 we extend our study to rooted forests. Recall that a graph is called a *forest* if it is a collection of tree components, or equivalently, it has no cycles. A tree is said to be *rooted* if a single node in that tree is designated as a root, and a *rooted forest* is a forest in which all trees are rooted. Let \mathcal{C} (resp., \mathcal{C}_k) denote the collection of all spanning rooted forests (consisting, resp., of k trees). Let us define the corresponding forest weights by

$$f(A) = \sum_{\pi \in \mathcal{C}} \prod_{e \in E(\pi)} a_e, \quad f_k(A) = \sum_{\pi \in \mathcal{C}_k} \prod_{e \in E(\pi)} a_e.$$

We show that, like the tree weight $t(A)$, each of $f_k(A)$, ($1 \leq k \leq n$) and $f(A)$ attain their maximum values at the uniform case A^* .

The formulas for $f_k(A)$ and $f(A)$ are used to show that the number of trees X_n in a random rooted forest (sampled with probability proportional to its weight) is *intrinsically divisible*, that is, representable as a sum of n independent Bernoulli random variables. More precisely, the success probability of the j th Bernoulli variable is $1/(1 + \lambda_j)$, where λ_j , ($1 \leq j \leq n$), are the eigenvalues of the *weighted* Kirchhoff matrix corresponding to A . With regard to this divisibility property, X_n is analogous to the number of sets in the random set partition [Harper (1967)], the number of edges in the random matching set [Heilmann and Lieb (1972), Godsil (1981)] and the number of pendant vertices in a random tree [Steele (1987)]. We illustrate applicability of the last result by showing that for the cube on $n = 2^k$ vertices, the random variable X_n is asymptotically Gaussian with mean and variance close to $2^k/k$.

2. Bounds on tree weight. The main results of this section are first, that on the set of all edge-weight distributions $A = [a_e]$ of a given total weight w , the tree weight function $t(A)$ attains its maximum at the uniform distribution $A^* = [a_e^* = w/N]$, $N = \binom{n}{2}$; and second, that a useful bound on $t(A)/t(A^*)$ can be formulated in terms of the vertex weights $a_i = \sum_{e \ni i} a_e$.

THEOREM 1.

$$\max \left\{ t(A) : \sum_e a_e = w \right\} = t(A^*) = \left(\frac{w}{N} \right)^{n-1} n^{n-2}.$$

THEOREM 2. For any weight distribution $A = [a_e]$,

$$t(A) \leq \frac{1}{n} \left(\frac{\sum a_i}{n-1} \right)^{n-1} \exp \left[\frac{n-1}{2(n-2)} - \frac{n-1}{2} \frac{\sum_{i=1}^n a_i^2}{(\sum a_i)^2} \right].$$

To prove the statements, first introduce the $n \times n$ Kirchhoff matrix $M = [m_{ij}(A)]$ associated with the weight distribution A :

$$(4) \quad m_{ij} = \begin{cases} -a_{(ij)}, & \text{if } i \neq j, \\ a_i, & \text{if } i = j. \end{cases}$$

Here are two well-known properties of M .

LEMMA 1. $M(A)$ is nonnegative definite.

PROOF. Let $x^{\text{tr}} = [x_1, \dots, x_n] \in R^n$. Then

$$\begin{aligned} x^{\text{tr}} M(A) x &= \sum_{i,j} a_{ij} x_i^2 - \sum_{i,j} a_{ij} x_i x_j \\ &= \frac{1}{2} \sum_{i,j} a_{ij} (x_i - x_j)^2 \\ &\geq 0. \end{aligned} \quad \square$$

Let $M_i(A)$ denote the cofactor of the (i, i) th element in $M(A)$. The following lemma is frequently called Maxwell's rule [Maxwell (1892)].

LEMMA 2. For each $i \in [n]$, $t(A) = M_i(A)$.

For a proof see, for instance, Moon (1970), Theorem 5.2. The next lemma is a well-known result about the average value of diagonal minors. See, for example, Godsil (1993).

LEMMA 3. Let $K \subset [n] = \{1, \dots, n\}$, let M be an $n \times n$ symmetric matrix with eigenvalues $\{\lambda_i\}$ and let M_K be the determinant of the $(n-k) \times (n-k)$ matrix obtained by deleting from M the rows and columns indexed in K . Then

$$\sum_{K \subset [n]: |K|=k} M_K = \sum_{J \subset [n]: |J|=n-k} \prod_{j \in J} \lambda_j.$$

PROOF OF THEOREM 1. Since $\mathbf{1} = [1, 1, \dots, 1]^{\text{tr}}$ is an eigenvector of $M = M(A)$ with eigenvalue 0, it follows from Lemma 1 that the smallest eigenvalue λ_n of M is 0. From Lemma 2 and Lemma 3 with $k = 1$,

$$\begin{aligned} t(A) &= \frac{1}{n} \sum_{i=1}^n \prod_{j \neq i} \lambda_j \\ &= \frac{1}{n} \prod_{i=1}^{n-1} \lambda_i \\ &\leq \frac{1}{n} \left(\frac{\text{tr}(M)}{n-1} \right)^{n-1} \end{aligned}$$

$$\begin{aligned}
 &= \frac{1}{n} \left(\frac{2w}{n-1} \right)^{n-1} \\
 &= t(A^*).
 \end{aligned}$$

This last equation can be seen either by noting that the eigenvalues of $M(A^*)$ are

$$\lambda_i^* = \frac{2w}{n-1}, \quad i = 1, \dots, n-1$$

and $\lambda_n^* = 0$, or by simply multiplying the number n^{n-2} of labelled trees by the common tree product

$$\left(\frac{2w}{n(n-1)} \right)^{n-1}. \quad \square$$

Note. The essential parts of Theorem 1 appear in several earlier works; see Grimmett (1976), Grone and Merris (1988). Nevertheless, Theorem 1 itself is not stated in any previous work that we have found.

PROOF OF THEOREM 2. As in the previous proof, let $\lambda_1 \geq \dots \geq \lambda_n = 0$ be the eigenvalues of the Kirchhoff matrix $M(A)$. Using Lemma 3 with $k = 2$, we get

$$\begin{aligned}
 \sum_{1 \leq i < j \leq n-1} \lambda_i \lambda_j &= \sum_{1 \leq i < j \leq n} \lambda_i \lambda_j \\
 &= \sum_{1 \leq i < j \leq n} (a_i a_j - a_{ij}^2) \\
 &\leq \sum_{1 \leq i < j \leq n} a_i a_j \\
 &= \frac{1}{2} \left[\left(\sum_i a_i \right)^2 - \sum_i a_i^2 \right].
 \end{aligned}$$

Next, applying the geometric–arithmetic mean inequality to $\binom{n-1}{2}$ numbers $\lambda_i \lambda_j$, we get

$$\left(\prod_{i=1}^{n-1} \lambda_i \right)^{n-2} = \prod_{1 \leq i < j \leq n-1} \lambda_i \lambda_j \leq \left[\frac{(\sum_i a_i)^2 - \sum_i a_i^2}{2 \binom{n-1}{2}} \right]^{\binom{n-1}{2}},$$

which implies

$$\begin{aligned}
 (5) \quad \prod_{i=1}^{n-1} \lambda_i &\leq \left(\frac{\sum_i a_i}{n-1} \right)^{n-1} \left(\frac{n-1}{n-2} \right)^{(n-1)/2} \left(1 - \frac{\sum_i a_i^2}{(\sum_i a_i)^2} \right)^{(n-1)/2} \\
 &\leq \left(\frac{\sum_i a_i}{n-1} \right)^{n-1} \exp \left(\frac{n-1}{2(n-2)} - \frac{n-1}{2} \frac{\sum_i a_i^2}{(\sum_i a_i)^2} \right),
 \end{aligned}$$

where the last inequality comes from $1 + x \leq e^x$. Finally, since $t(A) = (\prod_{i=1}^{n-1} \lambda_i)/n$, (5) implies the result of the theorem. \square

3. Application to spanning trees in sparse random graphs. Let $P = [p_e]$ be a symmetric matrix, with each entry $p_e \in [0, 1]$. Introduce the random graph model $\mathcal{G}(n, P)$ where edges appear independently and the probability of an edge e being present equals p_e , $e \in E(K_n)$. We will let G denote a realization of the random graph model \mathcal{G} . The special case in which $p_e \equiv p$ is referred to as the *uniform case*, and we denote it $\mathcal{G}(n, p)$. This case has been studied extensively since the 1950s, with works by Gilbert (1959), Kelmans (1972), Grimmett and McDiarmid (1975), Bollobás and Erdős (1976) and Stepanov (1970), to cite some examples.

A random graph model closely related to $\mathcal{G}(n, p)$ is the model $\mathcal{G}(n, m)$, in which a fixed number of edges $m = m(n)$ are distributed uniformly at random among all N positions. For many graph properties, these two models are asymptotically equivalent as $n \rightarrow \infty$ with $m = pN$, provided that $p(1-p)N = o((pN)^2)$, meaning that the variance of the number of edges in the random graph is negligible compared to its expected value. The model $\mathcal{G}(n, m)$ was the focus of Erdős and Rényi's cornerstone works (1959, 1960), and later Stepanov (1969) undertook a detailed study of $\mathcal{G}(n, p)$. An ever expanding bibliography of random graph literature may be traced through the texts by Bollobás (1985), Palmer (1985) and in a recent survey by Karoński (1995).

Of special interest is the case when the edge probability $p = c/n$ or $m = cn/2$, both conditions meaning that the average vertex degree is asymptotic to c . A major thrust of the Erdős–Rényi–Stepanov studies is that the random graph can be in one of the three phases, namely subcritical, nearcritical and supercritical, dependent on whether $c < 1$, c is close to 1 or $c > 1$. It is when c slightly exceeds 1 that the birth of a giant component takes place; see also Barbour (1982), Bollobás (1985), Pittel (1990), Janson, Knuth, Luczak and Pittel (1993), Luczak, Pittel and Wierman (1994).

Our focus here is primarily on the nonuniform sparse model, when $p_e = c_e/n$, and $c_e \not\equiv c$. With a notable exception of Stepanov (1970a, b) who studied the special case $p_{(ij)} = \alpha_i \alpha_j/n$, not much is known about the behavior of this random graph. Its analysis promises to be considerably more complicated since the classical graph-enumerating techniques can no longer be used freely.

In this section we investigate the probability that G , a random graph from the model $\mathcal{G}(n, [c_e/n])$, is a spanning tree. Let \mathcal{C} and $P(\mathcal{C})$ denote the set of all spanning trees on K_n and the probability in question. The probability that G is a given spanning tree $T \in \mathcal{C}$ is

$$\begin{aligned} P(T) &= \prod_{e \in E(T)} p_e \prod_{e' \notin E(T)} (1 - p_{e'}) \\ (6) \quad &= \prod_{e \in E(T)} \frac{p_e}{1 - p_e} \prod_{e' \in E(K_n)} (1 - p_{e'}). \end{aligned}$$

Clearly then,

$$\begin{aligned}
 (7) \quad P(\mathcal{L}) &= \sum_{T \in \mathcal{L}} P(T) \\
 &= t(A) \prod_{e \in E(K_n)} (1 - p_e),
 \end{aligned}$$

where

$$A \equiv \left[\frac{p_e}{1 - p_e} \right].$$

In the uniform case $[p_e = c/n]$, this probability simplifies to

$$\begin{aligned}
 P_0(\mathcal{L}) &= n^{n-2} (c/n)^{n-1} (1 - c/n)^{\binom{n}{2} - (n-1)} \\
 &\sim \frac{c^2}{n} (ce^{-c/2})^{n-3} \\
 &= O\left(\frac{2}{e}\right)^n.
 \end{aligned}$$

Our intent is to show, in the sparse case $[p_e] = [c_e/n]$ subject to some mild balancing restrictions on $[c_e]$, that $P(\mathcal{L})$ also approaches 0 exponentially fast, with the rate dominated by $P_0(\mathcal{L})$ in the sense that the relative risk $P(\mathcal{L})/P_0(\mathcal{L})$ is asymptotically bounded.

We assume that $[c_e]$ depends on n in such a way that

$$(8) \quad \limsup_{n \rightarrow \infty} \max_e p_e < 1,$$

and

$$\begin{aligned}
 &\lim_{n \rightarrow \infty} \bar{c} = \mu_c > 0, \\
 &\lim_{n \rightarrow \infty} N^{-1} \sum_e (c_e - \bar{c})^2 = \sigma_c^2 \geq 0, \\
 (9) \quad &\lim_{n \rightarrow \infty} n^{-1} \sum_{i=1}^n (\bar{c}_i - \bar{c})^2 = \nu_c^2 \geq 0 \quad \text{and} \\
 &\lim_{n \rightarrow \infty} (nN)^{-1} \sum_e |c_e - \bar{c}|^3 = 0.
 \end{aligned}$$

The meaning of (9) is that the sample mean and the sample variance of $[c_e]$ and also the sample variance of the vertex-associated averages $[\bar{c}_i] \equiv [\sum_{e \ni i} c_e / (n - 1)]$ all have finite limits. The generality of the conditions is in that, aside from the mild uniform restriction (8), they are of a global nature. In particular, we may regard the values $[c_e]$ as being realized from a random distribution with moment constraints given by (9).

THEOREM 3. Under conditions (8) and (9),

$$\limsup_{n \rightarrow \infty} \frac{P\{\mathcal{L}\}}{P_0\{\mathcal{L}\}} \leq \exp\left\{\sigma_c^2\left(\frac{1}{\mu_c} - \frac{1}{4}\right) - \frac{\nu_c^2}{2\mu_c^2}\right\}.$$

COROLLARY 1. For sufficiently large n , the uniform probability matrix $[p_e = \bar{c}/n]$ maximizes $P\{\mathcal{L}\}$ among all matrices satisfying conditions (8) and (9) with $\mu_c > 4$.

We begin by noticing that, according to (7),

$$(10) \quad \frac{P\{\mathcal{L}\}}{P_0\{\mathcal{L}\}} = \frac{t(A)}{t(A_0)} q_n,$$

$$(11) \quad q_n \equiv \frac{\prod_e (1 - p_e)}{(1 - \bar{p})^N}, \quad \bar{p} = \bar{c}/n$$

where

$$A_0 \equiv \left[\begin{array}{c} \bar{c}/n \\ 1 - \bar{c}/n \end{array} \right].$$

In view of (10), we need only to prove the following technical lemma.

LEMMA 4. Under conditions (8) and (9),

$$\limsup_{n \rightarrow \infty} \frac{t(A)}{t(A_0)} \leq \exp\left\{\frac{\sigma_c^2}{\mu_c} - \frac{\nu_c^2}{2\mu_c^2}\right\},$$

$$\lim_{n \rightarrow \infty} q_n = \exp\left\{\frac{-\sigma_c^2}{4}\right\}.$$

PROOF. From Theorem 2, we have

$$(12) \quad t(A) \leq \frac{1}{n} \left(\frac{\text{tr} M}{n-1} \right)^{n-1} \exp\left\{ \frac{n-1}{2(n-2)} - \frac{n-1}{2} \frac{\sum_{i=1}^n m_{ii}^2}{(\text{tr} M)^2} \right\},$$

where $M = [m_{ij}]$ is the Kirchhoff matrix for $A = [p_e/(1 - p_e)]$. Therefore,

$$(13) \quad \begin{aligned} \text{tr} M &= \sum_{i=1}^n \sum_{e \ni i} \frac{p_e}{1 - p_e} \\ &= 2 \sum_e \left(p_e + p_e^2 \frac{1}{1 - p_e} \right) \\ &= 2 \sum_e p_e + 2 \sum_e p_e^2 + O\left(\sum_e p_e^3 \right), \end{aligned}$$

the last equality following from (8). However, with $p_e = c_e/n$ and (9),

$$\begin{aligned} \sum_e p_e^3 &= \sum_e (p_e - \bar{p} + \bar{p})^3 \\ &= \frac{1}{n^3} \sum_e (c_e - \bar{c})^3 + \frac{3\bar{c}}{n^3} \sum_e (c_e - \bar{c})^2 + \binom{n}{2} \frac{\bar{c}^3}{n^3} \\ &= o(1). \end{aligned}$$

Therefore, (13) implies

$$\begin{aligned} \text{tr } M &= 2 \sum_e p_e + 2 \sum_e p_e^2 + o(1) \\ (14) \quad &= 2 \binom{n}{2} \frac{\bar{c}}{n} + \frac{2}{n^2} \sum_e c_e^2 + o(1) \\ &= (n-1) \left\{ \bar{c} + (nN)^{-1} \sum_e (c_e - \bar{c})^2 + \frac{\bar{c}^2}{n} \right\} + o(1), \end{aligned}$$

and thus

$$(15) \quad \frac{\text{tr } M}{n-1} = \bar{c} + (nN)^{-1} \sum_e (c_e - \bar{c})^2 + \frac{\bar{c}^2}{n} + o(n^{-1}).$$

We now express $\sum_i m_{ii}^2$ in terms of $[c_e]$. Observe that

$$\begin{aligned} m_{ii} &= \sum_{e \ni i} \frac{p_e}{1-p_e} \\ (16) \quad &= \frac{1}{n} \sum_{e \ni i} c_e + O\left(n^{-2} \sum_{e \ni i} c_e^2\right) \\ &= \bar{c}_i (1 + O(n^{-1})) + O\left(n^{-2} \sum_{e \ni i} c_e^2\right), \end{aligned}$$

since $\bar{c}_i = (\sum c_e)/(n-1)$; hence

$$(17) \quad m_{ii}^2 = \bar{c}_i^2 (1 + O(n^{-1})) + O\left(\bar{c}_i n^{-2} \sum_{e \ni i} c_e^2\right) + O\left(n^{-4} \left(\sum_{e \ni i} c_e^2\right)^2\right).$$

Now choose $\alpha \in (0, \frac{1}{2})$ and set $\beta = 2 - \alpha$. Applying the geometric–arithmetic mean inequality we have

$$\begin{aligned} 2\bar{c}_i n^{-2} \sum_{e \ni i} c_e^2 &= 2\bar{c}_i n^{-\alpha} n^{-\beta} \sum_{e \ni i} c_e^2 \\ (18) \quad &\leq \bar{c}_i^2 n^{-2\alpha} + n^{-2\beta} \left(\sum_{e \ni i} c_e^2\right)^2, \end{aligned}$$

and therefore

$$\begin{aligned}
 (19) \quad m_{ii}^2 &= \bar{c}_i^2(1 + O(n^{-1} + n^{-2\alpha})) + O\left((n^{-2\beta} + n^{-4})\left(\sum_{e \ni i} c_e^2\right)^2\right) \\
 &= \bar{c}_i^2(1 + O(n^{-2\alpha})) + O\left(n^{-2\beta}\left(\sum_{e \ni i} c_e^2\right)^2\right),
 \end{aligned}$$

since $2\alpha < 1$ and $2\beta < 4$. Then it follows that

$$(20) \quad \sum_{i=1}^n m_{ii}^2 = \sum_{i=1}^n \bar{c}_i^2 + O\left(n^{-2\alpha} \sum_{i=1}^n \bar{c}_i^2\right) + O\left(n^{-2\beta} \sum_{i=1}^n \left(\sum_{e \ni i} c_e^2\right)^2\right).$$

To bound the last term in (20), clearly

$$\begin{aligned}
 (21) \quad \sum_{i=1}^n \left(\sum_{e \ni i} c_e^2\right)^2 &\leq \left(2 \sum_e c_e^2\right)^2 \\
 &\leq \left(4 \sum_e (c_e - \bar{c})^2 + 2n^2 \bar{c}^2\right)^2 \\
 &\leq 16 \left(\sum_e (c_e - \bar{c})^2\right)^2 + 8 \left(\sum_e (c_e - \bar{c})^2\right) n^2 \bar{c}^2 + 4n^4 \bar{c}^4 \\
 &\leq 4n^4 \left[N^{-1} \sum_e (c_e - \bar{c})^2 + \bar{c}^4\right] \\
 &= O(n^4),
 \end{aligned}$$

the last estimate following from the second condition in (9). Combining (20) and (21),

$$\begin{aligned}
 (22) \quad \frac{1}{n-1} \sum_{i=1}^n m_{ii}^2 &= [1 + O(n^{-2\alpha})] \frac{1}{n-1} \sum_{i=1}^n \bar{c}_i^2 + O(n^{3-2\beta}) \\
 &= [1 + O(n^{-2\alpha})] \left[\frac{1}{n} \sum_{i=1}^n (\bar{c}_i - \bar{c})^2 + \bar{c}^2 \right] + O(n^{3-2\beta}).
 \end{aligned}$$

But $3 - 2\beta < 0$, and thus by (9), the limit of (22) as $n \rightarrow \infty$ is $\nu_c^2 + \mu_c^2$. The exponential term in (12) can now be evaluated completely:

$$\begin{aligned}
 (23) \quad &\exp\left\{ \frac{n-1}{2(n-2)} - \frac{n-1}{2} \frac{\sum_{i=1}^n m_{ii}^2}{(\text{tr } M)^2} \right\} \\
 &= \exp\left\{ \frac{n-1}{2(n-2)} - \frac{1}{2} \frac{\sum_{i=1}^n m_{ii}^2 / (n-1)}{(\text{tr } M / (n-1))^2} \right\} \\
 &\rightarrow \exp\left\{ \frac{1}{2} - \frac{\nu_c^2 + \mu_c^2}{2\mu_c^2} \right\} \\
 &= \exp\left\{ -\frac{\nu_c^2}{2\mu_c^2} \right\}.
 \end{aligned}$$

Recalling the definition of A_0 and (15), we obtain

$$\begin{aligned}
 & \frac{1}{n} \left(\frac{\text{tr} M}{n-1} \right)^{n-1} \frac{1}{t(A_0)} \\
 (24) \quad &= \frac{1}{n} \left[\bar{c} + \frac{1}{n} \left\{ N^{-1} \sum_e (c_e - \bar{c})^2 + \bar{c}^2 \right\} + o(n^{-1}) \right]^{n-1} \frac{(1 - \bar{c}/n)^{n-1}}{n^{n-2} (\bar{c}/n)^{n-1}} \\
 &= \left[1 + \frac{1}{n} \left\{ (\bar{c}N)^{-1} \sum_e (c_e - \bar{c})^2 + \bar{c} \right\} + o(n^{-1}) \right]^{n-1} (1 - \bar{c}/n)^{n-1}.
 \end{aligned}$$

Since $\bar{c} \rightarrow \mu > 0$, \bar{c} is asymptotically bounded away from 0, $o(n^{-1})/\bar{c} = o(n^{-1})$ and the above expression converges to

$$(25) \quad \exp \left\{ \frac{\sigma_c^2}{\mu_c} + \mu_c \right\} \exp \{-\mu_c\} = \exp \left\{ \frac{\sigma_c^2}{\mu_c} \right\}.$$

Therefore,

$$(26) \quad \limsup_{n \rightarrow \infty} \frac{t(A)}{t(A_0)} \leq \exp \left\{ \frac{\sigma_c^2}{\mu_c} - \frac{\nu_c^2}{2\mu_c^2} \right\}$$

holds.

Turning our attention to the asymptotic value of q_n , defined in (15), we may use condition (8) to write

$$\begin{aligned}
 \log q_n &= \sum_e \log \left(1 - \frac{c_e}{n} \right) - \binom{n}{2} \log \left(1 - \frac{\bar{c}}{n} \right) \\
 &= \sum_e \left[-\frac{c_e}{n} - \frac{c_e^2}{2n^2} + O\left(\frac{c_e^3}{n^3}\right) \right] - \binom{n}{2} \log \left(1 - \frac{\bar{c}}{n} \right) \\
 (27) \quad &= \binom{n}{2} \left[-\frac{\bar{c}}{n} - \frac{1}{2n^2} \sum_e c_e^2 + \frac{\bar{c}}{n} + \frac{\bar{c}^2}{2n^2} + O(n^{-3}) \right] + o(1) \\
 &= -\frac{1}{2n^2} \binom{n}{2} \left[\frac{1}{\binom{n}{2}} \sum_e c_e^2 - \bar{c}^2 \right] + O(n^{-1}) \\
 &\rightarrow -\frac{\sigma_c^2}{4}.
 \end{aligned}$$

Thus

$$(28) \quad \lim_{n \rightarrow \infty} q_n = \exp \left\{ \frac{-\sigma_c^2}{4} \right\},$$

and the lemma is proved. \square

PROOF OF THEOREM 3. Theorem 3 now follows easily from (10) and the limiting bounds (26) and (28):

$$(29) \quad \limsup_{n \rightarrow \infty} \frac{P\{\mathcal{L}\}}{P_0\{\mathcal{L}\}} = \limsup_{n \rightarrow \infty} \frac{t(A)}{t(A_0)} q_n \leq \exp\left\{\sigma_c^2 \left(\frac{1}{\mu_c} - \frac{1}{4}\right) - \frac{\nu_c^2}{2\mu_c^2}\right\}. \quad \square$$

The corollary now follows since σ_c^2 and ν_c^2 are nonnegative quantities.

Note. Having proved Theorem 3, we first thought that the uniform distribution might (asymptotically) maximize $P(\mathcal{L})$ for $[c_e]$ in a broader range of μ_c , perhaps even for $\mu_c > 1$. As the example below shows, however, if $[c_e]$ is subject to the restrictions (9) only, then the lower bound for μ_c cannot be pushed below $2 + \sqrt{2}$.

EXAMPLE 1. *Two-Component Graph.* Let $n = 2m$, $C = \{1, 2, \dots, m\}$, $\bar{C} = \{m+1, m+2, \dots, 2m\}$ and let c_1, c_2 be two positive constants. For $e = (i, j)$, set

$$c_e = \begin{cases} c_1, & \text{if } i \text{ and } j \text{ are both in the same component } C \text{ or } \bar{C}, \\ c_2, & \text{if } i \text{ and } j \text{ are in different components.} \end{cases}$$

An easy computation shows that, besides the zero eigenvalue, the Kirchoff matrix $M(A)$ with $A = [p_e/(1-p_e)]$ has an eigenvalue $m(a_1 + a_2)$ (of multiplicity $2m - 2$), and another eigenvalue $2ma_2$ (of multiplicity 1). Here

$$a_i = \frac{c_i/n}{1 - c_i/n}, \quad i = 1, 2.$$

It follows then from Lemma 2 and Lemma 3 that

$$t(A) \sim n^{-1} c_2 \left(\frac{c_1 + c_2}{2}\right)^{n-2} \exp\left(\frac{c_1^2 + c_2^2}{c_1 + c_2}\right), \quad n \rightarrow \infty.$$

The matrix $[c_e]$ satisfies (9) with

$$\mu_c = \frac{c_1 + c_2}{2}, \quad \sigma_c^2 = \frac{(c_1 - c_2)^2}{4}, \quad \nu_c = 0.$$

So, using (10) and the formula for $\lim q_n$ from Lemma 4, we obtain

$$P(\mathcal{L}) \sim n^{-1} c_2 \mu_c^{n-2} \exp\left(\frac{c_1^2 + c_2^2}{2\mu_c} - \frac{\sigma_c^2}{4}\right)$$

and

$$P_0(\mathcal{L}) \sim n^{-1} \mu_c^{n-1} \exp(\mu_c).$$

Taking the ratio and simplifying,

$$(30) \quad \begin{aligned} \lim_{n \rightarrow \infty} \frac{P(\mathcal{C})}{P_0(\mathcal{C})} &= \frac{c_2}{\mu_c} \exp \left[1 - \frac{c_2}{\mu_c} + \sigma_c^2 \left(\frac{1}{\mu_c} - \frac{1}{4} \right) \right] \\ &\leq \exp \left[\sigma_c^2 \left(\frac{1}{\mu_c} - \frac{1}{4} \right) \right], \end{aligned}$$

where the last inequality (expected according to our theorem) follows from $x e^{-x} \leq e^{-1}$. Notice that for $\rho \equiv \sigma_c/\mu_c$ small, the limiting ratio in (30) becomes

$$(31) \quad \exp \left[-\frac{\rho^2}{4} (\mu_c^2 - 4\mu_c + 2) + O(\rho^3) \right].$$

Thus, to guarantee that this quantity falls below 1, we need to have

$$\mu_c < 2 - \sqrt{2} \quad \text{or} \quad \mu_c > 2 + \sqrt{2}.$$

Thus, somewhat counterintuitively, the “bad” μ_c ’s fill the interval $[2 - \sqrt{2}, 2 + \sqrt{2}]$. We thought about a possibility to push the lower bound above $2 + \sqrt{2}$ by partitioning $[n]$ into $r > 2$ equal size blocks. Surprisingly, this didn’t change (31) and $2 + \sqrt{2}$ didn’t budge! Could it be that (31) is actually true for a much broader class of $[c_e]$?

Note. For any class \mathcal{C} of graphs on $[n]$, the random graph model $\mathcal{S}(n, P)$ induces a probability distribution of the form given in (1) with the graph π being represented by its adjacency matrix $R(\pi)$ and the canonical parameter matrix Θ having $(i, j) = e$ entry $\Theta_e = \log[P_{\mathcal{S}}(e)/(1 - P_{\mathcal{S}}(e))]$. In this case, the normalizing constant in (2) becomes $\psi(\Theta) \propto P_{\mathcal{S}}(\mathcal{C})$. The model derived from these choices in (1) gives the conditional probability under $\mathcal{S}(n, P)$ of a graph π given that $\pi \in \mathcal{C}$. In the remainder of the paper, we investigate $P_{\mathcal{S}}(\mathcal{C})$ for various classes \mathcal{C} of rooted forests. For such classes, we find a remarkable factorization of the model that takes the form of (1), but with $\Theta_e = \log P_{\mathcal{S}}(e)$.

4. Extension to forests. Recall some basic definitions: a tree is said to be *rooted* if it contains a specific node that is identified as a root. A *spanning forest* on the node set $[n]$ is a set of disjoint trees (some of which may be isolated nodes) whose node sets form a partition of $[n]$.

Let $K \subset [n]$ with $|K| = k$; let \mathcal{C}_K be the collection of spanning forests consisting of k trees, each rooted at one of the nodes in K and let $\mathcal{C}_k = \bigcup_{K \subset [n]} \mathcal{C}_K$. If a forest $\pi \in \mathcal{C}_k$ is represented by its $n \times n$ adjacency matrix $R(\pi)$, then, analogously to the tree weight, we define the *k-forest weight* f_k of $A = [a_e]$ by

$$(32) \quad f_k(A) = \sum_{\pi \in \mathcal{C}_k} \prod_{e \in E(\pi)} a_e.$$

Note that when $k = 1$, we have $f_1(A) = nt(A)$, where the factor n arises because a single tree on $[n]$ may be rooted at any of its n nodes.

Given $K \subset [n]$, let $f_K(A)$ denote the total weight of all forests of trees, each tree having exactly one vertex from K . [So $f_{[n]}(A) = t(A)$, in particular.] Then we may formulate the following theorem.

THEOREM 4.

$$f_K = M_K.$$

Consequently,

$$f_k(A) = \sum_{K \subset [n]: |K|=k} M_K(A),$$

where, we recall, $M_K(A)$ denotes the determinant of the submatrix of $M(A)$ with rows and columns indexed by the nodes from K^c .

Note. For $a_e \equiv 1$, the second relation can be read out from Biggs (1974), Chapter 6, Theorem 7.5. For the general case, Moon (1970) attributes the first relation (with $|K| = 2$) to Percival (1953). Our proof combines elements from Biggs and Moon.

PROOF. Let I be the $n \times N$ incidence matrix of K_n . Its rows are indexed by the nodes and the columns by the edges. A column labelled $e = (i, j)$ has two nonzero entries, $I_{ie} = -I_{je}$, both of unit absolute value. It is well known that I is unimodular; that is, all nonsingular square submatrices of I have their determinants equal to ± 1 . Introduce a reduced incidence matrix I_K obtained from I by deleting the rows labelled by the nodes from K .

LEMMA 5. *Let B be a square submatrix of order $n - k$ of I_K , where $k = |K|$. Then B is nonsingular if and only if:*

- (i) *the edges corresponding to the $(n - k)$ columns of B determine a spanning subforest of K_n that consists of k trees; and*
- (ii) *each of the k trees contains exactly one node from K .*

For a proof, see Biggs (1974), Chapter 2, Lemma 7.4.

Let D be a diagonal $N \times N$ matrix, with $D_{ee} = a_e$, and define $J_K = I_K D^{1/2}$. Then, applying the Binet–Cauchy theorem,

$$\begin{aligned} \det(I_K D I_K^{\text{tr}}) &= \det(J_K J_K^{\text{tr}}) \\ (33) \qquad \qquad \qquad &= \sum_{\mathcal{B}} \{\det \mathcal{B}\}^2; \end{aligned}$$

here the sum is over all $(n - k) \times (n - k)$ submatrices \mathcal{B} of J_K . Each such \mathcal{B} determines the corresponding submatrix B of I_K , so that

$$\det^2 \mathcal{B} = \left[\prod_e a_e \right] \det^2 B,$$

where the product is over all the edges $e \in E_B$ that correspond to the $(n - k)$ columns of B . Now, by Lemma 5, $|\det B| = 1$ or 0 , dependent upon whether the corresponding $(n - k)$ edges are the edges of a forest of k trees each having exactly one vertex from K . We conclude that

$$\det(I_K D I_K^{\text{tr}}) = f_K(A).$$

Finally, for $i \in K^c$,

$$\begin{aligned}
 (I_K DI_K^{\text{tr}})_{ii} &= \sum_{e \in E(K_n)} (I_K)_{ie} \alpha_e (I_K^{\text{tr}})_{ei} \\
 &= \sum_{e \in E(K_n)} [(I_K)_{ie}]^2 \alpha_e \\
 (34) \qquad &= \sum_{e \in E(K_n): e \ni i} \alpha_e \\
 &= m_{ii},
 \end{aligned}$$

and for $j \in K^c, j \neq i$,

$$\begin{aligned}
 (I_K DI_K^{\text{tr}})_{ij} &= \sum_{e \in E(K_n)} (I_K)_{ie} \alpha_e (I_K^{\text{tr}})_{ej} \\
 (35) \qquad &= \sum_{e \in E(K_n)} (I_K)_{ie} (I_K)_{je} \alpha_e \\
 &= -\alpha_{(i, j)}.
 \end{aligned}$$

Therefore,

$$\det(I_K DI_K^{\text{tr}}) = \det[m_{ij}]_{i, j \in K^c} = M_K. \quad \square$$

The following is a generalization of Theorem 1 to the forest weight.

THEOREM 5. $\max\{f_k(A) : \sum_e \alpha_e = w\} = f_k(A^*) = (w/N)^{n-k} \binom{n}{k} kn^{n-k-1}$.

PROOF. Recall that

$$\begin{aligned}
 f_k(A) &= \sum_{K \subset N: |K|=k} M_K(A) \\
 &= \sum_{J \subset N: |J|=n-k} \prod_{j \in J} \lambda_j,
 \end{aligned}$$

where the λ 's are the eigenvalues of the Kirchoff matrix for the weighted adjacency matrix A . But $f_k(A)$ is a Schur concave function on $\{\lambda_1, \dots, \lambda_{n-1}\}$ (recall $\lambda_n = 0$) [see, e.g., Marshall and Olkin (1979), page 61]. Hence

$$\begin{aligned}
 \sum_{J \subset N: |J|=n-k} \prod_{j \in J} \lambda_j &\leq \binom{n-1}{n-k} \left(\frac{\sum_{i=1}^n \lambda_i}{n-1} \right)^{n-k} \\
 (36) \qquad &= \binom{n-1}{n-k} \left(\frac{\text{tr}(M)}{n-1} \right)^{n-k} \\
 &= \left(\frac{w}{N} \right)^{n-k} \binom{n}{k} kn^{n-k-1}.
 \end{aligned}$$

The inequality on line one becomes the equality in the uniform case $A^* = [w/N]$. \square

Let $f(A)$ denote the total weight of all forests of rooted trees, that is,

$$f(A) = \sum_{k=1}^n f_k(A).$$

COROLLARY 2. $\max\{f(A): \sum_e a_e = w\} = f(A^*) = (1 + wn/N)^{n-1}$.

For the general edge-weight distribution, summing both sides of the equation

$$f_k(A) = \sum_{J \subset N: |J|=n-k} \prod_{j \in J} \lambda_j$$

from $k = 1$ to n , we get

$$\begin{aligned} (37) \quad f(A) &= \prod_{j=1}^n (1 + \lambda_j) = \prod_{j=1}^{n-1} (1 + \lambda_j) \\ &= \det(I_n + M(A)). \end{aligned}$$

Note. Chung and Langlands (1996) [see also Chung (1997)] proved (for unit edge weights) that the number of rooted forests spanning an induced subgraph equals the product of its vertex degrees and the Dirichlet eigenvalues of the corresponding Laplacian operator. With the vertex degrees replaced by the vertex weights, the corresponding formula would certainly hold for the weighted case, too. If we consider K_n as a subgraph of K_{n+1} , with each of the extra n edges being of unit weight, then (37) is a consequence of that general identity.

5. On the intrinsic divisibility of the number of rooted trees in a random forest. Formula (37) leads to a surprisingly concise description of the distribution of the number of tree components in a random spanning forest generated from model (1). That is, suppose we pick a forest of rooted trees with probability proportional to its weight. Then p_k , the probability that the random forest consists of k (rooted) trees is given by

$$p_k = \frac{\sum_{J: |J|=n-k} \prod_{j \in J} \lambda_j}{\prod_{j=1}^n (1 + \lambda_j)}.$$

Consequently, the probability generating function (p.g.f.) of X , the number of trees in the forest, is

$$\begin{aligned} E[x^X] &= \frac{\sum_{k=1}^n x^k \sum_{J: |J|=n-k} \prod_{j \in J} \lambda_j}{\prod_{j=1}^n (1 + \lambda_j)} \\ &= \frac{\prod_{j=1}^n (x + \lambda_j)}{\prod_{j=1}^n (1 + \lambda_j)} \\ &= \prod_{j=1}^n \left(\frac{\lambda_j}{1 + \lambda_j} + x \frac{1}{1 + \lambda_j} \right). \end{aligned}$$

This formula means that X has the same distribution as the sum of n independent, binary random variables ε_j , with

$$\Pr(\varepsilon_j = 0) = 1 - \Pr(\varepsilon_j = 1) = \frac{\lambda_j}{1 + \lambda_j}.$$

Thus the number of trees in the random rooted forest possesses what we would like to call an intrinsic divisibility property. Among previously discovered random variables with this property are the number of blocks in a random set partition [Harper (1967)], the number of edges in the random matching set [Heilmann and Lieb (1972), Godsil (1981)], the number of edges common for a fixed edge set and the random spanning tree [Godsil (1984)] and the number of leaves in a random tree [Steele (1987)]. The distribution of the latter turned out to be intimately connected to that of the number of blocks in Harper (1967). Jeff Kahn (1997) has pointed out to us that our result could also have been obtained from that of Godsil (1984), via the embedding of K_n into K_{n+1} . For a highly readable survey of the area, the reader is referred to Pitman (1997). In it probabilistic methods are used to get strong bounds on the coefficients of polynomials whose roots are all real. In our case where the roots are non-negative, it is well-known that the coefficient sequence is unimodal.

Whenever intrinsic divisibility is established, it quickly leads to various results, including the asymptotic behavior of the distribution in question; see Harper (1967), Godsil (1981) and Kahn (1996), for instance. In our case, since

$$\begin{aligned} \text{Var } X &= \sum_{j=1}^n \Pr(\varepsilon_j = 0) \Pr(\varepsilon_j = 1) \\ &= \sum_{j=1}^n \frac{\lambda_j}{(1 + \lambda_j)^2}, \end{aligned}$$

we obtain: if the matrix A changes with $n \rightarrow \infty$ in such a way that

$$\sum_{j=1}^n \frac{\lambda_j}{(1 + \lambda_j)^2} \rightarrow \infty,$$

then $(X - E[X])/\text{Var}^{1/2} X$ converges, in distribution, to the standard normal variable [Durrett (1991)].

EXAMPLE 2. Consider the d -dimensional cube Q_d . Assume that all its $d2^{d-1}$ edges are of unit weight. The nonzero eigenvalues of the Kirchhof matrix in this case are $2m$ of multiplicity $\binom{d}{m}$, ($1 \leq m \leq d$) [see Chung (1997)]. Let X_d be the number of trees in a random rooted forest which spans Q_d . Then, using standard tricks, we obtain

$$\begin{aligned} EX_d &= \sum_{j=1}^{2^d-1} \frac{1}{1 + \lambda_j} \\ &= \sum_{m=1}^d \binom{d}{m} \frac{1}{1 + 2m} \\ (38) \qquad &= \frac{2^d}{d} (1 + O(d^{-1})); \end{aligned}$$

$$\begin{aligned}\text{Var } X_d &= \sum_{j=1}^{2^d-1} \frac{\lambda_j}{(1 + \lambda_j)^2} \\ &= \sum_{m=1}^d \binom{d}{m} \frac{2m}{(1 + 2m)^2} \\ &= \frac{2^d}{d} (1 + O(d^{-1})).\end{aligned}$$

Thus we can claim that $(X_d - \mathbb{E}X_d) \text{Var}^{-1/2} X_d$ converges, in distribution, to the standard normal variable. As a weak consequence of this result we can claim that almost all trees in the random spanning forest are of order d , the dimension of the cube.

Although it might seem plausible that the number of trees in a random forest of *unrooted* trees is also representable as a sum of binary random variables, this is easily seen not to be the case, since for $n = 3$ the corresponding p.g.f. is $(x^3 + 3x^2 + 3x)/7$, which has complex roots.

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