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On Generalized Zagreb Indices of Random Graphs

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Abstract

Random graphs play an important role in the study of graph theory. The two most common models are $G(n,p)$ and $G(n,m)$ random graphs. In this paper, we first introduce a graphic polynomial analogous to the degree sequence polynomial and use it to compute the expected values of generalized first Zagreb indices for $G(n,p)$ random graphs. Then we turn to $G(n,m)$ random graphs and employ a different method to compute the expected values of the first Zagreb index and of the forgotten index. Using the same approach we also compute the expected values of the second Zagreb index for both considered classes of random graphs. We validate our results by comparing them with results of numerical simulations conducted over wide range of parameters.

1 Introduction

Let G be a graph with the vertex set $V(G)$ and the edge set $E(G)$. In this paper we consider the simple graphs (graphs with no loops and no multiple edges). For a vertex $v \in V(G)$, the degree of v is denoted by $d(v)$. *Adjacency matrix* of a graph G of order n, $A = [a_{ij}]$, is an $n \times n$ matrix, where $a_{ij} = 1$ if $v_i v_j \in E(G)$, and $a_{ij} = 0$, otherwise.

The study of random graphs is one of the most important areas of graph theory. Random graphs have found many applications in natural and social sciences. For example, they are used as a standard null model in simulating many physical processes on graphs and networks, see [21, 22]. For some early applications we refer the reader to [2, 7, 16] and for more recent development see, for example, [1, 5, 15, 17, 18]. We find particularly striking Kauffman's speculations about the origins of life via the emergence of a giant component in auto-catalytic chemical networks.

A random graph is obtained by starting with a set of isolated vertices and adding successive edges between them at random. There are different random graph models produced by different probability distributions on graphs. Most commonly studied is the one denoted by $G(n, p)$, consisting of all labeled graphs on n vertices in which every possible edge occurs independently with probability $0 < p < 1$, see [3,4]. Another natural model of random graphs has the probability space $G(n, m)$ consisting of all labeled graphs on n vertices and m edges. The random graphs $G(n, m)$ were studied by Erdős and Rényi in their pioneering work on the evolution of random graphs [8,9]. Note that every random graph in $G(n, p)$ gives a random symmetric $(0, 1)$-matrix such that each entry above the main diagonal with probability p is equal 1, and vice versa. Also, every random graph in $G(n, m)$ gives a random symmetric $(0, 1)$-matrix which contains exactly m entries 1 above the main diagonal, and vice versa. Hence, the study of these random graphs is equivalent to the study of related random symmetric $(0, 1)$-matrices.

A *graph invariant* is a numerical quantity which is uniquely determined for a graph and is invariant under graph isomorphism. Graph invariants are extensively used in chemistry as molecular descriptors. In chemical graph theory, several degree-based graph invariants have been considered and applied in the studies. Among them, the *first Zagreb index* M_1 and the *second Zagreb index* M_2 are among the oldest and most thoroughly investigated, see [12, 20]. For a graph G they are defined as follows:

$$M_1(G) = \sum_{uv \in E(G)} d(u) + d(v) = \sum_{v \in V(G)} d^2(v) \quad \text{and} \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v) \ .$$

The sum of cubes of vertex degrees of a graph G in [10] is called the *forgotten topological index* and denoted by $F(G)$, i.e.,

$$F(G) = \sum_{uv \in E(G)} d^2(u) + d^2(v) = \sum_{v \in V(G)} d^3(v) \ .$$

Also the physico-chemical applications of $F(G)$ have been investigated in [10]. The forgotten index is just one of a series of similarly defined indices. The *ℓ-th generalized first Zagreb index* $M_1^\ell(G)$ is defined [19] as the sum of ℓ-th powers of degrees of vertices of G,

$$M_1^\ell(G) = \sum_{u \in V(G)} d_u^\ell \ .$$

Hence, $M_1^1(G) = 2|E(G)|$ and $M_1^2(G) = M_1(G)$, while for $\ell = 3$ one obtains the forgotten index $F(G)$.

Let G be a graph with the degree sequence $\delta = d_1 \leq \ldots \leq d_m = \Delta$. Its *degree sequence polynomial* $S_G(x)$ is defined as the generating polynomial of its degree sequence in [25], i.e., as

$$S_G(x) = \sum_{u \in V(G)} x^{d_u} = \sum_{j=\delta}^{\Delta} a_j x^j \ ,$$

where a_j denotes the number of vertices of degree j. The evaluations of the polynomial and its first derivative at 1 give, respectively, the number of vertices and twice the number of edges of G. Hence, $S_G(1) = |V(G)|$ and $S'_G(1) = 2|E(G)|$.

For $G \in G(n,p)$, let D_u be a random variable corresponding to the degree of vertex $u \in V(G)$. Its vertex degree distribution is given by

$$\mathbb{P}(D_u = k) = \binom{n-1}{k} p^k (1-p)^{n-1-k}.$$

Now, we define a polynomial function

$$f_{(n,p)}(x) = \sum_{k=0}^{n-1} \binom{n-1}{k} (1-p)^{n-1-k} p^k x^k = (1 - p + px)^{n-1} \ .$$

It can be easily verified by direct computation that the j-th derivative of $f_{(n,p)}(x)$ evaluated at $x = 1$ has the following form:

$$f_{(n,p)}^{(j)}(1) = (n-1)\cdot\ldots\cdot(n-j)p^j,$$

for all $1 \leq j \leq n-1$.

It was shown in [6] that the degree sequence polynomial encodes all information necessary for computing generalized first Zagreb indices of arbitrary order. The same is valid for our polynomial $f_{(n,p)}(x)$. This information is extracted using a family of combinatorial numbers known as Stirling numbers of the second kind.

The *Stirling numbers of the second kind*, denoted by $\left\{ {n \atop k} \right\}$, count, among other things, the number of partitions of a set of n elements into k non-empty subsets. They satisfy a linear recurrence,

$$\left\{ {n \atop k} \right\} = k\left\{ {n-1 \atop k} \right\} + \left\{ {n-1 \atop k-1} \right\}$$

for $n > 0$, with the initial conditions $\left\{ {0 \atop 0} \right\} = 1$ and $\left\{ {0 \atop j} \right\} = \left\{ {i \atop 0} \right\} = 0$, for all $i, j \neq 0$. We refer the reader to [11] for a detailed exposition of these numbers and their properties. The most important for our purpose is the fact that the Stirling numbers of the second kind are used to convert between powers and falling factorials,

$$x^n = \sum_k \left\{ {n \atop k} \right\} x^{\underline{k}},$$

where $x^{\underline{k}}$ is the falling factorial defined as $x^{\underline{k}} = x(x-1)\ldots(x-k+1)$. The opposite relationship,

$$x^{\underline{n}} = \sum_k \left[{n \atop k} \right] (-1)^{n-k} x^k,$$

involves the Stirling numbers of the first kind $\left[{n \atop k} \right]$ that count the ways to arrange n objects into cycles. Here we quote the main result in [6]:

Theorem A. [6] *Let G be a simple connected graph and $S_G(x)$ its degree sequence polynomial. Then the ℓ-th general Zagreb index of G can be computed as*

$$M_1^{\ell}(G) = \sum_{j=1}^{\ell} \left\{ {\ell \atop j} \right\} S_G^{(j)}(1)$$

for any $\ell \in \mathbb{N}$.

Another way of looking at Zagreb indices is via matrix products. Let j be the vector of all ones. For a random graph G with adjacency matrix A (equivalently, for a random symmetric $(0,1)$-matrix A), the following holds.

$$M_1(G) = D \cdot D$$

where $D = Aj$ is a vector whose entries are the degrees of vertices of G and "$\cdot$" denotes the standard inner product of vectors. Also, let $Z = (z_1, \ldots, z_n)^T$ be a real column vector and let $B = [b_{ij}]$ be a real matrix of order n. One can find that

$$Z^T B Z = \sum_{1 \le p,q \le n} b_{pq} z_p z_q.$$

Hence, for a random graph G with adjacency matrix A (equivalently, for a random symmetric $(0,1)$-matrix A),

$$M_2(G) = \frac{1}{2} D^T A D.$$

For a random graph G with the vertex set $V(G) = \{v_1, \ldots, v_n\}$, we consider the *indicator random variables* X_{ij}, $1 \le i,j \le n$, defined by:

$$X_{ij} = \begin{cases} 1 & \text{if } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

So $X_{ij} = X_{ji}$ and since we only consider simple random graphs, $X_{ii} = 0$. Notice that if $G \in G(n,p)$, then the indicator random variables X_{ij} and X_{rs} are independent, where $1 \le i,j,r,s \le n$ and $\{i,j\} \ne \{r,s\}$. On the other hand, if $G \in G(n,m)$, then the indicator random variables X_{ij}, where $1 \le i,j \le n$, are not independent. The average value (or mean) of a random variable X is called its *expectation*, and is denoted by $\mathbb{E}(X)$. It is known that when X and Y are independent random variables, $\mathbb{E}(XY) = \mathbb{E}(X)\mathbb{E}(Y)$, see [24]. Also if X is an indicator random variable, then $\mathbb{E}(X^k) = \mathbb{E}(X)$, for each $k > 0$.

In [13, 14], the variance and the covariance of some degree-based graph invariants of random graphs $G(n,p)$ were studied in the special cases $p = \frac{\alpha(n-1)}{\binom{n}{2}}$ and $p = \frac{\alpha}{n}$, respectively, for a fixed parameter $\alpha > 0$. In this paper, we study the expectation of the first and the second Zagreb indices and the forgotten index of $G(n,p)$ and $G(n,m)$ random graphs.

2 Generalized first Zagreb indices of $G(n,p)$ random graphs

In this section, the polynomial $f_{(n,p)}(x)$ is used to obtain compact formulas for the expected values of all generalized Zagreb indices of $G(n,p)$ random graphs.

Theorem 1. *Let $G \in G(n,p)$ and $n \geq \ell + 1$. Then*

$$\mathbb{E}(M_1^\ell(G)) = n \sum_{j=1}^{\ell} \left\{ {\ell \atop j} \right\} \frac{n!}{(n-j-1)!} p^j.$$

Proof. Let D_u be the random variable corresponding to the degree of vertex $u \in V(G)$.

$$\begin{aligned}
\mathbb{E}(M_1^\ell(G)) &= \mathbb{E}\left(\sum_{u \in V(G)} D_u^\ell \right) = \sum_{u \in V(G)} \mathbb{E}\left(D_u^\ell\right) \\
&= \sum_{u \in V(G)} \sum_{k=0}^{n-1} k^\ell \binom{n-1}{k} p^k (1-p)^{n-1-k} \\
&= \sum_{u \in V(G)} \sum_{k=0}^{n-1} \sum_{j=1}^{\ell} \left\{ {\ell \atop j} \right\} k^{\underline{j}} \binom{n-1}{k} p^k (1-p)^{n-1-k} \\
&= \sum_{u \in V(G)} \sum_{j=1}^{\ell} \left\{ {\ell \atop j} \right\} \sum_{k=0}^{n-1} k^{\underline{j}} \binom{n-1}{k} p^k (1-p)^{n-1-k}.
\end{aligned}$$

The innermost sum evaluates to $(n-1) \cdot \ldots \cdot (n-j)p^j$, and our claim follows. ■

In Theorem 1, by setting $p = 1$ one readily recovers the known result for complete graphs, $\mathbb{E}(M_1^\ell(K_n)) = n(n-1)^\ell$. Also, Theorem 1 can be expressed in a more compact form in terms of our polynomial $f_{(n,p)}(x)$.

Corollary 2. *Let $G \in G(n,p)$ and $n \geq \ell + 1$. Then*

$$\mathbb{E}(M_1^\ell(G)) = n \sum_{j=1}^{\ell} \left\{ {\ell \atop j} \right\} f_{(n,p)}^{(j)}(1).$$

For the ordinary first Zagreb index and for the forgotten index, we specialize $\ell = 2$ and $\ell = 3$, respectively, and obtain the following expressions.

Corollary 3. *Let $G \in G(n,p)$ and $n \geq 3$. Then*

$$\mathbb{E}\left(M_1(G)\right) = n(n-1)p\left[(n-2)p + 1\right].$$

Corollary 4. *Let $G \in G(n,p)$ and $n \geq 4$. Then*

$$\mathbb{E}\left(F(G)\right) = n(n-1)p + 3n(n-1)(n-2)p^2 + n(n-1)(n-2)(n-3)p^3.$$

3 The first Zagreb index and the forgotten index of $G(n,m)$ random graphs

As we have already mentioned, the indicator random values X_{ij} are not independent for $G(n,m)$ random graphs. Hence, we cannot employ the same proof technique as in the $G(n,p)$ case. Instead, in this and in the next section, for two positive integers n and m, we define the parameters p_i, $i=1,2,3$, as follows:

$$p_i = \frac{\binom{\binom{n}{2}-i}{m-i}}{\binom{\binom{n}{2}}{m}} = \frac{m(m-1)\cdots(m-i+1)}{\binom{n}{2}(\binom{n}{2}-1)\cdots(\binom{n}{2}-i+1)}.$$

Here we do not look at the general ℓ, but only at the cases $\ell=2$ and $\ell=3$.

Theorem 5. *Let $G \in G(n,m)$ and $n \geq 3$. Then*

$$\mathbb{E}\left(M_1(G)\right) = n(n-1)\left(p_1 + (n-2)p_2\right).$$

Proof. Let $V(G) = \{v_1, \ldots, v_n\}$. Also let the random variable $D_i = \sum_{\substack{k=1\\k\neq i}}^{n} X_{ik}$ be corresponding to the degree of the vertex v_i, $i=1,\ldots,n$. Thus

$$\begin{aligned}
\mathbb{E}\left(M_1(G)\right) &= \mathbb{E}\left(\sum_{v_i \in V(G)} D_i^2\right) = \sum_{i=1}^{n} \mathbb{E}\left(D_i^2\right) = \sum_{i=1}^{n} \mathbb{E}\left((\sum_{\substack{k=1\\k\neq i}}^{n} X_{ik})^2 \right) \\
&= \sum_{i=1}^{n} \mathbb{E}\left(\sum_{\substack{k=1\\k\neq i}}^{n} X_{ik}^2\right) + \sum_{i=1}^{n} \mathbb{E}\left(\sum_{\substack{k=1\\k\neq i}}^{n} \sum_{\substack{r=1\\r\neq i,k}}^{n} X_{ik}X_{ir}\right) \\
&= \sum_{i=1}^{n} \sum_{\substack{k=1\\k\neq i}}^{n} \mathbb{E}\left(X_{ik}^2\right) + \sum_{i=1}^{n} \sum_{\substack{k=1\\k\neq i}}^{n} \sum_{\substack{r=1\\r\neq i,k}}^{n} \mathbb{E}\left(X_{ik}X_{ir}\right) \\
&= n(n-1)p_1 + n(n-1)(n-2)p_2,
\end{aligned}$$

and the proof is completed. ■

Theorem 6. *Assume that $G \in G(n,m)$ and $n \geq 4$. Then the following holds.*

$$\mathbb{E}\left(F(G)\right) = n(n-1)\left(p_1 + 3(n-2)p_2 + (n-2)(n-3)p_3\right).$$

Proof. As before, for a graph G with vertex set $V(G) = \{v_1, \ldots, v_n\}$, let D_i be the random variable corresponding to the degree of v_i, $i = 1, \ldots, n$. Then,

$$\begin{aligned}
\mathbb{E}\left(F(G)\right) &= \mathbb{E}\left(\sum_{v_i \in V(G)} D_i^3\right) = \sum_{i=1}^{n} \mathbb{E}\left(D_i^3\right) = \sum_{i=1}^{n} \mathbb{E}\left((\sum_{\substack{k=1 \\ k\neq i}}^{n} X_{ik})^3 \right) \\
&= \sum_{i=1}^{n} \mathbb{E}\left(\sum_{\substack{k=1 \\ k\neq i}}^{n} X_{ik}^3\right) + 3\sum_{i=1}^{n}\sum_{\substack{k=1 \\ k\neq i}}^{n} \mathbb{E}\left(X_{ik}^2 \left(\sum_{\substack{r=1 \\ r\neq i,k}}^{n} X_{ir}\right)\right) \\
&\quad + \sum_{i=1}^{n} \mathbb{E}\left(\sum_{\substack{k=1 \\ k\neq i}}^{n}\sum_{\substack{r=1 \\ r\neq i,k}}^{n}\sum_{\substack{s=1 \\ s\neq i,k,r}}^{n} X_{ik}X_{ir}X_{is}\right) \\
&= \sum_{i=1}^{n}\sum_{\substack{k=1 \\ k\neq i}}^{n} \mathbb{E}\left(X_{ik}^3\right) + 3\sum_{i=1}^{n}\sum_{\substack{k=1 \\ k\neq i}}^{n}\left(\sum_{\substack{r=1 \\ r\neq i,k}}^{n} \mathbb{E}\left(X_{ik}^2 X_{ir}\right)\right) \\
&\quad + \sum_{i=1}^{n}\sum_{\substack{k=1 \\ k\neq i}}^{n}\sum_{\substack{r=1 \\ r\neq i,k}}^{n}\sum_{\substack{s=1 \\ s\neq i,k,r}}^{n} \mathbb{E}\left(X_{ik}X_{ir}X_{is}\right) \\
&= n(n-1)p_1 + 3n(n-1)(n-2)p_2 + n(n-1)(n-2)(n-3)p_3
\end{aligned}$$

and we are done. ■

We observe that the results of Theorems 5 and 6 have the same structure as the results of Corollaries 3 and 4, respectively. Each of them could be converted to the other by switching between p^i and p_i, for $i = 1, 2, 3$. Hence, we are inclined to believe that the expected values of all generalized first Zagreb indices of $G(n, m)$ graphs could be expressed in a way analogous to the one established in Theorem 1. We have not worked out the details due to difficulties with expressing in a compact form the sums of products of binomial coefficients that arise along the way.

4 Second Zagreb indices of $G(n, p)$ and $G(n, m)$ random graphs

In this section, we compute the expectation of the second Zagreb index for random graphs in $G(n, p)$ and in $G(n, m)$.

Theorem 7. *Consider a graph $G \in G(n, p)$ such that $n \geq 3$. Then*

$$\mathbb{E}\left(M_2(G)\right) = \binom{n}{2}\left(p + 2(n-2)p^2 + (n-2)^2p^3\right).$$

Proof. Let $V(G) = \{v_1, \ldots, v_n\}$ and D_i be the random variable corresponding to the degree of v_i, $i = 1, \ldots, n$. Hence, the expectation of the second Zagreb index of G can be obtained as follows.

$$\mathbb{E}\left(M_2(G)\right) = \mathbb{E}\left(\sum_{v_iv_j \in E(G)} D_iD_j\right) = \frac{1}{2}\mathbb{E}\left(\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} D_iD_jX_{ij}\right) = \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} \mathbb{E}\left(D_iD_jX_{ij}\right). \quad (1)$$

In the last summation of the equations in (1), consider the term $\mathbb{E}\left(D_iD_jX_{ij}\right)$ for the fixed distinct positive integers i and j.

$$\begin{aligned}
\mathbb{E}\left(D_iD_jX_{ij}\right) &= \sum_{\substack{k=1\\k\neq i}}^{n}\sum_{\substack{r=1\\r\neq j}}^{n} \mathbb{E}\left(X_{ik}X_{jr}X_{ij}\right) \qquad (2)\\
&= \mathbb{E}\left(X_{ij}X_{ji}X_{ij}\right) + \sum_{\substack{k=1\\k\neq i,j}}^{n} \mathbb{E}\left(X_{ik}\right)\mathbb{E}\left(X_{ji}X_{ij}\right)\\
&\quad + \sum_{\substack{r=1\\r\neq j,i}}^{n} \mathbb{E}\left(X_{jr}\right)\mathbb{E}\left(X_{ij}X_{ij}\right) + \sum_{\substack{k=1\\k\neq i,j}}^{n}\sum_{\substack{r=1\\r\neq j,i}}^{n} \mathbb{E}(X_{ik})\mathbb{E}(X_{jr})\mathbb{E}(X_{ij})\\
&= p + 2(n-2)p^2 + (n-2)^2p^3.
\end{aligned}$$

Now, combining the equations in (1) and (2) yields the following relations.

$$\begin{aligned}
\mathbb{E}\left(M_2(G)\right) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} \mathbb{E}\left(D_iD_jX_{ij}\right)\\
&= \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} \left(p + 2(n-2)p^2 + (n^2-2n)p^3\right)\\
&= \frac{1}{2}(n^2-n)\left(p + 2(n-2)p^2 + (n-2)^2p^3\right)
\end{aligned}$$

which gives the result. ■

Theorem 8. *If $G \in G(n,m)$ and $n \geq 3$, then*

$$\mathbb{E}\left(M_2(G)\right) = \binom{n}{2}\left(p_1 + 2(n-2)p_2 + (n-2)^2p_3\right).$$

Proof. Consider the graph G with the vertex set $V(G) = \{v_1, \ldots, v_n\}$. As before, suppose that D_i is a random variable corresponding to the degree of v_i, $i = 1, \ldots, n$. Hence, the expectation of the second Zagreb index of G can be obtained as:

$$\mathbb{E}\left(M_2(G)\right) = \mathbb{E}\left(\sum_{v_iv_j \in E(G)} D_iD_j\right) = \frac{1}{2}\mathbb{E}\left(\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} D_iD_jX_{ij}\right) = \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n} \mathbb{E}\left(D_iD_jX_{ij}\right). \quad (3)$$

On the other hand, for the fixed distinct positive integers i, j, the term $\mathbb{E}\left(D_iD_jX_{ij}\right)$ in the last equation can be computed as follows.

$$\begin{aligned}\mathbb{E}\left(D_iD_jX_{ij}\right) &= \sum_{\substack{k=1\\k\neq i}}^{n}\sum_{\substack{r=1\\r\neq j}}^{n}\mathbb{E}\left(X_{ik}X_{jr}X_{ij}\right) \\ &= \mathbb{E}\left(X_{ij}X_{ji}X_{ij}\right)+\sum_{\substack{k=1\\k\neq i,j}}^{n}\mathbb{E}\left(X_{ik}X_{ji}X_{ij}\right) \\ &\quad+\sum_{\substack{r=1\\r\neq j,i}}^{n}\mathbb{E}\left(X_{jr}X_{ij}X_{ij}\right)+\sum_{\substack{k=1\\k\neq i,j}}^{n}\sum_{\substack{r=1\\r\neq j,i}}^{n}\mathbb{E}(X_{ik}X_{jr}X_{ij}) \\ &= p_1+2(n-2)p_2+(n-2)^2p_3.\end{aligned} \tag{4}$$

Now, combining the equations in (3) and (4) yields the following relations.

$$\begin{aligned}\mathbb{E}\left(M_2(G)\right) &= \frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n}\mathbb{E}\left(D_iD_jX_{ij}\right)=\frac{1}{2}\sum_{i=1}^{n}\sum_{\substack{j=1\\j\neq i}}^{n}\left(p_1+2(n-2)p_2+(n-2)^2p_3\right) \\ &= \frac{1}{2}(n^2-n)\left(p_1+2(n-2)p_2+(n-2)^2p_3\right)\end{aligned}$$

as desired. ■

Again, we observe that the results of Theorems 7 and 8 have the same structure – one can be obtained from the other by switching between p^i and p_i for $i = 1, 2, 3$. Also, note if $G \in G(n, p)$ or $G \in G(n, m)$ such that $p = 1$ and $m = \binom{n}{2}$ (consequently $p_i = 1$, $i = 1, 2, 3$), then G is the complete graph K_n and the results in Sections 3, 4 give the first and the second Zagreb index and the forgotten index of the such graph.

5 Computational results

In this section we report some computations for variety of random graphs, with the aim of comparing the results obtained in this paper with the experimental results obtained using Sage Mathematics Software System [26]. At first, for some positive integers n, m and rational number $0 \leq p \leq 1$, we generated 10000 random graphs in $G(n, p)$ and $G(n, m)$, for each special case of n, m and p. Next, we computed the mean of exact values of the first and the second Zagreb indices and the forgotten index of generated random graphs (which are denoted by "mean( )" in the tables) and then, we compared them with the expectation of the related graph invariants which are obtained in Theorems and Corollaries $1-8$ (and are denoted by "$\mathbb{E}$( )" in the tables). In Table 1, this comparison has been done for random graphs in $G(30,p)$, where $p \in \{0.3, 0.5, 0.7, 0.9\}$. Also, in Table 2, this comparison has been done for random graphs in $G(30,m)$, such that $m \in \{50, 100, 200, 300, 400\}$.

$G = G(n,p)$	$G(30,0.3)$	$G(30,0.5)$	$G(30,0.7)$	$G(30,0.9)$
mean$(M_1(G))$	2455.4974	6523.4010	12537.5340	20523.4836
$\mathbb{E}\,(\mathrm{M}_1(\mathrm{G}))$	2453.4000	6525.0000	12545.4000	20514.6000
mean$(M_2(G))$	11547.0998	48918.6361	129097.4064	268916.0004
$\mathbb{E}\,(\mathrm{M}_2(\mathrm{G}))$	11530.9800	48937.5000	129217.6200	268741.2600
mean$(F(G))$	24634.2406	100879.0722	261778.4260	539810.1270
$\mathbb{E}\,(\mathrm{F}(\mathrm{G}))$	24596.6400	100920.0000	262016.1600	539455.6800

Table 1: Comparison of experimental results and the expectation of some degree-based graph invariants for random graphs in $G(n,p)$.

$G = G(n,m)$	$G(30,50)$	$G(30,100)$	$G(30,200)$	$G(30,300)$	$G(30,400)$
mean$(M_1(G))$	415.7564	1477.6814	5534.8100	12174.2032	21393.6556
$\mathbb{E}\,(\mathrm{M}_1(\mathrm{G}))$	416.1290	1477.4193	5535.4838	12174.1935	21393.5483
mean$(M_2(G))$	855.4970	5426.9531	38202.3663	123393.5258	286001.4608
$\mathbb{E}\,(\mathrm{M}_2(\mathrm{G}))$	856.7496	5425.0391	38212.0688	123392.7512	285998.7484
mean$(F(G))$	1989.9814	11844.4328	79181.6314	250393.5204	573670.6496
$\mathbb{E}\,(\mathrm{F}(\mathrm{G}))$	1994.5839	11838.3818	79211.2940	250394.0847	573662.1023

Table 2: Comparison of experimental results and the expectation of some degree-based graph invariants for random graphs in $G(n,m)$.

We have also computed the expected values of generalized first Zagreb indices for random graphs in $G(n,n-1)$ and for random trees trying to determine their asymptotics for large ℓ. In all cases the expected values are linear in the number of edges $n-1$. For $G(n,n-1)$ random graphs, we find that the quantity $\mathbb{E}(M^{\ell}(G))/(n-1)$ behaves as the sequence $1, 2, 6, 22, 94, 454, \ldots$ for small values of $\ell \geq 0$. The sequence seem to be the sequence A001861 from the On-Line Encyclopedia of Integer Sequences [23]. The sequence has the exponential generating function given by $e^{2(e^x-1)}$, and among its combinatorial representations are the values of Bell polynomials and moments of the Poisson distribution with mean equal to 2. For random trees T on n vertices, $\mathbb{E}(M^{\ell}(T))/(n-1)$ seems to behave like the sequence of Bell numbers, A00110 of [23], that starts as $1, 2, 5, 15, 52, \ldots$. It would be interesting to provide combinatorial explanation for the observed behavior of the leading coefficients of the sequences of expected values.

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