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Estrada index of dynamic random graphs

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Abstract. The Estrada index of a graph G on n vertices is defined by $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the adjacency eigenvalues of G. We define two general types of dynamic graphs evolving according to continuous-time Markov processes with their stationary distributions matching the Erdös-Rényi random graph and the random graph with given expected degrees, respectively. We formulate some new estimates and upper and lower bounds for the Estrada indices of these dynamic graphs.

§1 Introduction

Let $G = (V, E)$ be a simple graph on vertex set $V = \{1, 2, \cdots, n\}$ with $|V| = n$ and edge set $E \subseteq V \times V$. The adjacency matrix of G is a binary matrix denoted by $A(G) = (a_{ij}) \in \mathbb{R}^{n\times n}$, where $a_{ij} = a_{ji} = 1$ if vertices i and j are adjacent, and $a_{ij} = a_{ji} = 0$ otherwise. As G is an undirected graph, $A(G)$ is symmetric and its n eigenvalues can be arranged in the non-increasing order $\lambda_1(A(G)) \geq \lambda_2(A(G)) \geq \cdots \geq \lambda_n(A(G))$; see e.g. [4].

The Estrada index of a graph G, defined by

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i(A(G))},$$

is a graph spectral invariant put forward by Estrada [6] in the year 2000. Abundant applications of Estrada index have been found in biochemistry and complex networks including quantifying the degree of folding of long-chain molecules [7, 10, 11] as well as network resilience metrics [15, 16]. Upper and lower bounds and varied mathematical properties have been examined for Estrada index and its close variants, see [1, 2, 5, 8, 12, 17, 18] to name a few.

Most of the existing work in this field has focused on static graphs. However, almost all real networks have vertices or edges appearing or disappearing as the network topology evolves with time. In [17], the present author proposed a calculation scheme for Estrada index in dealing with evolving graphs, where the dynamic graph is taken as a set of ordered snapshots of network architecture. The results are further extended to study Laplacian Estrada index and

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normalized Laplacian Estrada index in [18]. The snapshots in these works, nevertheless, are taken as independent measurements of the dynamic graph and the strong correlations between them are overlooked. This potentially ignored a wealth of hidden information in the evolving system.

In this paper, following this line of research, we aim to study the Estrada index of a couple of dynamic graphs where the edges appear and disappear following continuous-time Markov processes. By doing so, the entire history of the graph, instead of uncorrelated individual snapshots, is taken into consideration. The models considered here are fairly general in the sense that the edges in the graph are allowed to change with heterogeneous time-dependent rates. Moreover, the stationary distributions of these dynamical graph models can be viewed as classical Erdös-Rényi random graph [9] and random graph with given expected degrees [3], respectively. In this sense, our results also extend the Estrada index result of random graphs [2]. By considering these dynamic random graphs, we are able to track the change of Estrada index at each time instant rather than only presenting an overall "average" index for a sequence of deterministic graphs as in the previous work [17, 18].

We mention that dynamic graphs modeled by Markov chains akin to our models have been developed extensively in statical physics; see, e.g. [14]. However, the focus of these works is often on the topological and behavioral properties of dynamic processes over the networks and statistical data fitting. The rest of the paper is organized as follows. The main theoretical results together with illustrative computer simulations are presented in Section 2. We conclude the paper in Section 3.

§2 Main results

In this section, we estimate the Estrada index EE of two dynamic random graph models. To this end, we will use standard Landau asymptotic notations. For example, for two functions $f(n)$ and $g(n)$, $f(n) = o(g(n))$ implies that $\lim_{n\to\infty} f(n)/g(n) = 0$; $f(n) = O(g(n))$ means that $|f(n)/g(n)| \leq C$ for some constant C and sufficiently large n. A property for a random graph model holds asymptotically almost surely (a.a.s.) if its probability tends to 1 as $n \to \infty$.

2.1 Estrada index for dynamic random graphs

We first consider a simple dynamic random graph model, in which the appearance and disappearance of each edge following a continuous-time Markov process with identical rates. In the next section, we will extend this assumption to heterogeneous rates.

Given any pair of vertices, for $t \geq 0$ define $\lambda(t)$ to be the rate of the appearance of an edge between these two vertices where previously it is not there. Similarly, define $\mu(t)$ to be the rate of disappearance of an existing edge between these two vertices. Let $p_0(t)$ and $p_1(t)$ be the probabilities that there is no edge and one edge, respectively, between the given pair of vertices at time t. Therefore, we have the master equation

$$\frac{dp_1(t)}{dt} = \lambda(t)p_0(t) - \mu(t)p_1(t) = -\frac{dp_0(t)}{dt}. \tag{1}$$

Given the initial graph at time $t = 0$, we call this dynamic graph model $G_n(\lambda(t), \mu(t), t)$. Recall that the Erdös-Rényi random graph $G_n(p)$, on the other hand, is a static random graph where each edge appears independently with probability p.

Theorem 1. *Let $G_n(\lambda(t), \mu(t), t)$ $(t \geq 0)$ be a dynamic random graph. We have the following.*

(i) For $t \geq 0$, $EE(G_n(\lambda(t), \mu(t), t)) = \exp\big(Cne^{-\int_0^t(\lambda(s)+\mu(s))ds} + n\int_0^t \lambda(s)e^{-\int_s^t(\lambda(u)+\mu(u))du} ds\big) \cdot (e^{O(\sqrt{n})} + o(1))$, a.a.s., where $C = 0$ if the initial graph at time $t = 0$ is an empty graph and $C = 1$ if it is a complete graph.

(ii) Suppose $\lambda(t) \equiv \lambda$ and $\mu(t) \equiv \mu$. For any initial graph,

$$\lim_{t\to\infty} EE(G_n(\lambda, \mu, t)) = EE\Big(G_n\Big(\frac{\lambda}{\lambda+\mu}\Big)\Big) = e^{\frac{\lambda n}{\lambda+\mu}} \cdot (e^{O(\sqrt{n})} + o(1)) \quad a.a.s.$$

Proof. (i) By the definition of the dynamic random graph $G_n(\lambda(t), \mu(t), t)$, we have $p_0(t) + p_1(t) = 1$ for all $t \geq 0$. This together with (1) yields the solution

$$p_1(t) = Ce^{-\int_0^t(\lambda(s)+\mu(s))ds} + \int_0^t \lambda(s)e^{-\int_s^t(\lambda(u)+\mu(u))du} ds, \tag{2}$$

where the constant C is determined by the initial condition of the edge in question. If the edge is not present at $t = 0$, then $p_1(0) = 0$ and hence $C = 0$. If the edge is present at $t = 0$, then $p_1(0) = 1$ and hence $C = 1$.

Since the Markov processes on each edge have the same rates and run independently, $G_n(\lambda(t), \mu(t), t)$ is a random graph with edge probability $p_1(t)$. In view of the result [2, Theorem 2.3] that $EE(G_n(p)) = e^{np}(e^{O(\sqrt{n})} + o(1))$ a.a.s., we obtain by (2)

$$\begin{aligned} EE(G_n(\lambda(t), \mu(t), t)) =& e^{np_1(t)}(e^{O(\sqrt{n})} + o(1)) \\ =& \exp\Big(Cne^{-\int_0^t(\lambda(s)+\mu(s))ds} + n\int_0^t \lambda(s)e^{-\int_s^t(\lambda(u)+\mu(u))du} ds\Big) \\ &\cdot (e^{O(\sqrt{n})} + o(1)), \end{aligned}$$

where $C = 0$ if the initial graph is an empty graph and $C = 1$ if it is a complete graph.

(ii) When $\lambda(t) \equiv \lambda$ and $\mu(t) \equiv \mu$, the solution (2) for any edge reduces to

$$p_1(t) = \frac{\lambda}{\lambda+\mu} - C'e^{-(\lambda+\mu)t},$$

where $C' = \frac{\lambda}{\lambda+\mu} - C$. In the limit of $t \to \infty$, the probability of an edge between any pair of vertices $p_1(t) \to \frac{\lambda}{\lambda+\mu}$. Note that $EE(G_n(\lambda, \mu, t))$ is a continuous function with respect to t. Hence,

$$\lim_{t\to\infty} EE(G_n(\lambda, \mu, t)) = EE\Big(G_n\Big(\frac{\lambda}{\lambda+\mu}\Big)\Big) = e^{\frac{\lambda n}{\lambda+\mu}} \cdot (e^{O(\sqrt{n})} + o(1)) \quad a.a.s.$$

by applying again Theorem 2.3 in [2]. □

Remark 1. Assume $\lambda(t) \equiv \lambda$, $\mu(t) \equiv \mu$ and the initial graph is empty. By (i) we derive

$$EE(G_n(\lambda, \mu, t)) = e^{\frac{\lambda n}{\lambda+\mu}(1-e^{-(\lambda+\mu)t})} \cdot (e^{O(\sqrt{n})} + o(1)) \quad a.a.s. \tag{3}$$

for all $t \geq 0$. Moreover, the stationary distribution of the dynamic random graph model $G_n(\lambda, \mu, t)$ is simply the Erdös-Rényi random graph $G_n(p)$ with $p = \frac{\lambda}{\lambda+\mu}$.

To illustrate the theoretical result, we consider a dynamic graph $G_n(\lambda, \mu, t)$ with the initial graph at $t = 0$ as an empty graph. The probability of having an edge between any pair of vertices at $t = 1$ is given by $p_1(1) = a := \frac{\lambda}{\lambda+\mu}(1 - e^{-\lambda-\mu})$ through applying (2) and $C = 0$. Likewise, if initially the edge is present then the probability of disappearance of this edge at $t = 1$ is $p_0(1) = b := \frac{\mu}{\lambda+\mu}(1 - e^{-\lambda-\mu})$ through solving (2) with $C = 1$ and $p_0(1) = 1 - p_1(1)$. With these probabilities, we can conveniently model the dynamic random graph in discrete observation time as follows. Start with an empty graph at $t = 0$. At time $t + 1$, each edge appears with probability a if it does not exist at time t. Similarly, each edge disappears with probability b if it exists at time t. It is direct to check that the limit probability $\frac{\lambda}{\lambda+\mu} = \frac{a}{a+b}$.

In Fig. 1, we show the logarithmic Estrada index $lnEE(G_n(\lambda, \mu, t))$ for a dynamic random graph with $\lambda = 1$ and $\mu = 2$ over $n = 5000$ vertices. The initial graph is chosen as an empty graph. We observe that the behavior of $lnEE(G_n(\lambda, \mu, t))$ is consistent with the theoretical result (3).

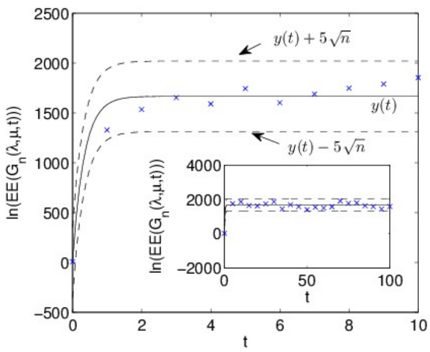

Figure 1. Logarithmic Estrada index $lnEE(G_n(\lambda, \mu, t))$ for dynamic graph with $\lambda = 1$, $\mu = 2$, $n = 5000$. We define $y(t) = \frac{\lambda n}{\lambda+\mu}(1 - e^{-(\lambda+\mu)t})$ and the observation time interval is $\Delta t = 1$. The blue crosses are the data points. Inset: the same result (with observation time interval $\Delta t = 5$) displayed over a larger time span.

2.2 Estrada index for dynamic random graphs with given expected degrees

Given n vertices and a sequence $\mathbf{w} = (w_1, w_2, \cdots, w_n)$, the well-known random graph with given expected degrees [3], denoted by $G_n(\mathbf{w})$, is defined by connecting each pair of vertices i and j with probability $\frac{w_i w_j}{\sum_{l=1}^n w_l}$ independently. Note that loops and multi-edges are allowed but their presence does not play any essential role. The expected degree of each vertex i is w_i in this static model. The Erdös-Rényi random graph $G_n(p)$ can be viewed as a special case of $G_n(\mathbf{w})$ with $w_i = np$ for all i.

Here, we consider a dynamic version of this model. For $t \geq 0$ we consider the Poisson process where each of the existing edges in the graph is deleted independently at rate μ, and for any pair of vertices i and j, edges between them are added at rate λ. Note that there can be k ($k \geq 0$) edges connecting each pair of vertices, and k is incremented at the rate λ but decremented at the rate $k\mu$. Let $p_k(t)$ be the probability that a given pair of vertices has k

edges at time t. Thus, we have the master equation

$$\frac{dp_k(t)}{dt} = \lambda p_{k-1}(t) + (k+1)\mu p_{k+1}(t) - \lambda p_k(t) - k\mu(t) p_k(t). \tag{4}$$

Given the initial graph at time $t = 0$, we call this dynamic graph model $G_n(\lambda, \mu, \mathbf{w}, t)$. In the following, we will focus on a special situation where $\lambda = \mu \frac{w_i w_j}{\sum_{l=1}^n w_l}$. In this case, the stationary distribution of $G_n(\lambda, \mu, \mathbf{w}, t)$ is the same as the static random graph model with given expected degrees $G_n(\mathbf{w})$ (see below).

Let $\Delta = \max_{1 \le l \le n} w_l$. We have the following estimates for the Estrada index of $G_n(\lambda, \mu, \mathbf{w}, t)$.

Theorem 2. *Let $G_n(\lambda, \mu, \mathbf{w}, t)$ $(t \ge 0)$ be a dynamic random graph with given expected degrees. Assume $\Delta \gg \ln^4 n$ and $\lambda = \mu \frac{w_i w_j}{\sum_{l=1}^n w_l}$ for any pair of vertices i and j. We have the following.*

(i) For $t \ge 0$, $e^{-(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^n e^{\lambda_l(\overline{A})} \le EE(G_n(\lambda, \mu, \mathbf{w}, t)) \le e^{(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^n e^{\lambda_l(\overline{A})}$ a.a.s., where $\overline{A} = (p_{ij}) \in \mathbb{R}^{n \times n}$ with $p_{ij} = \frac{w_i w_j}{\sum_{l=1}^n w_l}(1 - e^{-\mu t})$ if there is no edge between vertices i and j in the initial graph at time $t = 0$, while $p_{ij} = \frac{w_i w_j}{\sum_{l=1}^n w_l} + \exp\big(-\mu t - \frac{w_i w_j}{\sum_{l=1}^n w_l}\big)\big(1 - \frac{2 w_i w_j}{\sum_{l=1}^n w_l}\big)$ if there is an edge between vertices i and j in the initial graph.

(ii) For any initial graph, $e^{-(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^n e^{\lambda_l(\overline{A})} \le \lim_{t \to \infty} EE(G_n(\lambda, \mu, \mathbf{w}, t)) = EE(G_n(\mathbf{w})) \le e^{(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^n e^{\lambda_l(\overline{A})}$ a.a.s., where $\overline{A} = (p_{ij}) \in \mathbb{R}^{n \times n}$ with $p_{ij} = \frac{w_i w_j}{\sum_{l=1}^n w_l}$.

Proof. (i) Fix a pair of vertices i and j. Define a probability generating function $H(x, t) = \sum_{k=0}^\infty p_k(t) x^k$. Drawing on the master equation (4) and $\lambda = \mu \frac{w_i w_j}{\sum_{l=1}^n w_l}$, we derive

$$\frac{\partial H(x,t)}{\partial t} = (x-1)\mu \cdot \Big(\frac{w_i w_j}{\sum_{l=1}^n w_l} H(x,t) - \frac{\partial H(x,t)}{\partial x}\Big).$$

Since $H(1, t) = 1$, it can be checked easily that the solution is

$$H(x,t) = \exp\Big(\frac{w_i w_j}{\sum_{l=1}^n w_l}(x-1)\Big)\varphi((x-1)e^{-\mu t}), \tag{5}$$

where $\varphi(x)$ is any once-differentiable function satisfying $\varphi(0) = 1$ determined by the initial condition. If there is no edge between vertices i and j at $t = 0$, we have $p_0(0) = 1$ and $p_k(0) = 0$ for $k \ge 1$. We have $H(x, 0) = 1$ and from (5) if follows that $\varphi(x) = \exp\big(-\frac{w_i w_j x}{\sum_{l=1}^n w_l}\big)$. The average number of edges between vertices i and j is given by

$$\frac{\partial H(x,t)}{\partial x}\Big|_{x=1} = \frac{w_i w_j}{\sum_{l=1}^n w_l} + e^{-\mu t}\varphi'(0) = \frac{w_i w_j}{\sum_{l=1}^n w_l}(1 - e^{-\mu t}).$$

We denote this value by p_{ij}. Similarly, if there is one edge between vertices i and j at $t = 0$, we have $p_0(0) = 0$, $p_1(0) = 1$ and $p_k(0) = 0$ for $k \ge 2$. Hence, $H(x, 0) = x$ and it follows from (5) that $\varphi(x) = (x+1)\exp\big(-\frac{w_i w_j x}{\sum_{l=1}^n w_l}\big)$. The average number of edges between vertices i and j is given by

$$p_{ij} := \frac{\partial H(x,t)}{\partial x}\Big|_{x=1} = \frac{w_i w_j}{\sum_{l=1}^n w_l} + e^{-\mu t}\varphi'(0) = \frac{w_i w_j}{\sum_{l=1}^n w_l} + e^{-\mu t - \frac{w_i w_j}{\sum_{l=1}^n w_l}}\Big(1 - \frac{2 w_i w_j}{\sum_{l=1}^n w_l}\Big).$$

The same expressions hold for each pair of vertices in the graph depending on the initial condition, i.e., whether the edge exists or not at $t = 0$.

At any $t \ge 0$, $G_n(\lambda, \mu, \mathbf{w}, t)$ can be viewed as an edge-independent random graph with mean number of edges p_{ij} on a pair of vertices i and j. Since $\Delta \gg \ln^4 n$, from Theorem 1 [13], it follows readily that the eigenvalues can be estimated as $|\lambda_i(A(G_n(\lambda,\mu,\mathbf{w},t))) - \lambda_i(\overline{A})| \le (2+o(1))\sqrt{\Delta}$ a.a.s. for each $i = 1,\cdots,n$, where $\overline{A} = (p_{ij}) \in \mathbb{R}^{n\times n}$. Therefore,

$$\lambda_i(\overline{A}) - (2+o(1))\sqrt{\Delta} \le \lambda_i(A(G_n(\lambda,\mu,\mathbf{w},t))) \le \lambda_i(\overline{A}) + (2+o(1))\sqrt{\Delta} \quad a.a.s.$$

Based on the definition of Estrada index, we obtain

$$e^{-(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^{n} e^{\lambda_l(\overline{A})} \le EE(G_n(\lambda,\mu,\mathbf{w},t)) \le e^{(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^{n} e^{\lambda_l(\overline{A})} \quad a.a.s.$$

(ii) For any initial graph at $t = 0$, in the limit of $t \to \infty$, the average number of edges between any vertices i and j tends to $p_{ij} = \frac{w_i w_j}{\sum_{l=1}^{n} w_l}$, implying that the stationary state of the model is the static random graph with given expected degrees $G_n(\mathbf{w})$. Since $EE(G_n(\lambda,\mu,\mathbf{w},t))$ is continuous with respect to t, the result of (i) gives rise to $e^{-(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^{n} e^{\lambda_l(\overline{A})} \le \lim_{t\to\infty} EE(G_n(\lambda,\mu,\mathbf{w},t)) = EE(G_n(\mathbf{w})) \le e^{(2+o(1))\sqrt{\Delta}} \cdot \sum_{l=1}^{n} e^{\lambda_l(\overline{A})}$ a.a.s., where $\overline{A} = (p_{ij}) \in \mathbb{R}^{n\times n}$. This completes the proof. □

§3 Conclusion

We have studied Estrada index of two classes of dynamic random graphs, which can be viewed as generalizations of static Erdös-Rényi random graph and random graph with given expected degrees, respectively. The evolution of graph follows continuous-time Markov processes with general heterogeneous time-varying rates. Some interesting directions for future work include extension to other relevant graph-theoretical metrics such as the Laplacian Estrada index. Another appealing open problem is to consider both edge dynamics and vertex dynamics in the graph evolution as well as more general random graph models [19,20], which characterize many realistic large-scale networks.

Declarations

Conflict of interest The authors declare no conflict of interest.

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