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ESTRADA INDEX OF ITERATED LINE GRAPHS

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A b s t r a c t. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a graph G, then the Estrada index of G is $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$. If $L(G) = L^1(G)$ is the line graph of G, then the iterated line graphs of G are defined as $L^k(G) = L(L^{k-1}(G))$ for $k = 2, 3, \ldots$. Let G be a regular graph of order n and degree r. We show that $EE(L^k(G)) = a_k(r)\, EE(G) + n\, b_k(r)$, where the multipliers $a_k(r)$ and $b_k(r)$ depend only on the parameters r and k. The main properties of $a_k(r)$ and $b_k(r)$ are established.

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1. *Introduction*

Let G be a graph of order n. The eigenvalues of the adjacency matrix of G, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$, are said to be the eigenvalues of G, and they form the spectrum of G [3]. As well known [3], the spectra of graphs have found numerous applications in various fields of science. One of the newest such application was put forward by Ernesto Estrada, who arrived at the conclusion that the graph–spectrum–based graph invariant

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

can be used as a measure of the degree of folding of long–chain polymeric molecules, especially those of biological importance [5, 6, 7]. Somewhat later, Estrada and Rodríguez–Velázquez used the same quantity EE to describe certain properties (so-called "centrality") of complex networks [9, 10]; some most recent results along these lines can be found in [8]. In what follows, EE will be called *the Estrada index*.

The study of the mathematical properties of the Estrada index started only quite recently [4, 11, 12], and relatively little is known on its dependence on the structure of the underlying graph. In this work we report on the properties of the Estrada index of iterated line graphs of regular graphs.

Let, as usual, $L(G)$ denote the line graph of the graph G. For $k = 1, 2, \ldots$, the k-th iterated line graph of G is defined as $L^k(G) = L(L^{k-1}(G))$, where $L^0(G) = G$ and $L^1(G) = L(G)$.

If G is a regular graph of degree $r = 0$, then $L^k(G)$, $k \geq 1$, are graphs without vertices. In this case, $EE(G) = n$ and $EE(L^k(G)) = 0$ for $k \geq 1$. If G is a regular graph of degree $r = 1$, then $L(G)$ consists of isolated vertices, and $L^k(G)$, $k \geq 2$, are graphs without vertices. In this case, $EE(G) = (n/2)(e+1/e)$, $EE(L(G)) = n/2$, and $EE(L^k(G)) = 0$ for $k \geq 2$. If G is a regular graph of degree $r = 2$, then $L(G) \cong G$ and, consequently, $L^k(G) \cong G$ for all $k \geq 1$. In this case, $EE(L^k(G)) = EE(G)$ for all $k \geq 1$. Therefore, in order to avoid these trivial cases, in what follows we assume that the degree r of the regular graphs considered is at least three.

The line graph of a regular graph G of order $n = n_0$ and of degree $r = r_0$ is a regular graph of order $n_1 = nr/2$ and of degree $r_1 = 2r - 2$. Consequently, all the iterated line graphs of a regular graph are regular graphs. In particular, the order n_k and degree r_k of $L^k(G)$, $k \geq 1$, obey the recurrence relations

$$n_k = \frac{1}{2}\, n_{k-1}\, r_{k-1} \quad ; \quad r_k = 2\, r_{k-1} - 2 \tag{2}$$

from which one directly obtains [1, 2]:

$$r_k = 2^k\, r - 2^{k+1} + 2 \tag{3}$$

$$n_k = \frac{n}{2^k} \prod_{i=0}^{k-1} r_i = \frac{n}{2^k} \prod_{i=0}^{k-1} \left(2^i\, r - 2^{i+1} + 2\right) . \tag{4}$$

For the sake of simplicity we define

$$\gamma_k(r) := \begin{cases} 1 & \text{for } k=0 \\ \dfrac{1}{2^k} \displaystyle\prod_{i=0}^{k-1} \left(2^i\, r - 2^{i+1} + 2\right) & \text{for } k \geq 1 \end{cases} \tag{5}$$

and then Eq. (4) can be rewritten as

$$n_k = \gamma_k(r)\, n \ . \tag{6}$$

Both Eqs. (3) and (6) hold for $k \geq 0$.

According to a classical result of Sachs [13], if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a regular graph G of order n and of degree r, then the eigenvalues of its line graph $L(G)$ are

$$\left.\begin{array}{lll} \lambda_i + r - 2 & i = 1, 2, \ldots, n & \text{and} \\ -2 & n(r-2)/2 \quad \text{times} \ . & \end{array}\right\} \tag{7}$$

Combining formulas (1) and (7) one immediately arrives at

Lemma 1. *If G is a regular graph of order n and degree $r \geq 3$, then the Estrada indices of G and $L(G)$ are related as*

$$EE(L(G)) = e^{r-2}\, EE(G) + \frac{r-2}{2\,e^2}\, n \ . \tag{8}$$

Lemma 2. *If $G = L^0(G)$ is a regular graph of order $n = n_0$ and degree $r = r_0 \geq 3$, then for $k \geq 0$, the Estrada indices of $L^k(G)$ and $L^{k+1}(G)$ are related as*

$$EE(L^{k+1}(G)) = e^{r_k-2}\, EE(L^k(G)) + \frac{r_k-2}{2\,e^2}\, n_k \ . \tag{9}$$

Evidently, for $k = 0$, Eq. (9) reduces to Eq. (8). It should be noted that Eqs. (8) and (9) hold also in the cases $r = 0, 1, 2$.

By a two-fold application of Lemma 2 we get

$$\begin{aligned} EE(L^2(G)) &= e^{r_1-2}\, EE(L^1(G)) + \frac{r_1-2}{2\,e^2}\, n_1 \\ &= e^{r_1-2} \left[e^{r_0-2}\, EE(L^0(G)) + \frac{r_0-2}{2\,e^2}\, n_0 \right] + \frac{r_1-2}{2\,e^2}\, n_1 \ , \end{aligned}$$

i.e.,

$$EE(L^2(G)) = e^{r_1-2}\, e^{r_0-2}\, EE(L^0(G)) + e^{r_1-2}\, \frac{r_0-2}{2\,e^2}\, n_0 + \frac{r_1-2}{2\,e^2}\, n_1 \ . \quad (10)$$

In a similar manner,

$$\begin{aligned} EE(L^3(G)) &= e^{r_2-2}\, e^{r_1-2}\, e^{r_0-2}\, EE(L^0(G)) + e^{r_2-2}\, e^{r_1-2}\, \frac{r_0-2}{2\,e^2}\, n_0 \\ &+ e^{r_2-2}\, \frac{r_1-2}{2\,e^2}\, n_1 + \frac{r_2-2}{2\,e^2}\, n_2 \end{aligned} \quad (11)$$

$$\begin{aligned} EE(L^4(G)) &= e^{r_3-1}\, e^{r_2-2}\, e^{r_1-2}\, e^{r_0-2}\, EE(L^0(G)) + e^{r_3-2}\, e^{r_2-2}\, e^{r_1-2}\, \frac{r_0-2}{2\,e^2}\, n_0 \\ &+ e^{r_3-2}\, e^{r_2-2}\, \frac{r_1-2}{2\,e^2}\, n_1 + e^{r_3-2}\, \frac{r_2-2}{2\,e^2}\, n_2 + \frac{r_3-2}{2\,e^2}\, n_3 \ . \end{aligned} \quad (12)$$

It is not difficult to see that Eqs. (10)–(12) are special cases of the formula:

$$EE(L^{k+1}(G)) = \left(\prod_{i=0}^{k} e^{r_i-2}\right) EE(G) + \sum_{p=0}^{k-1} \left(\prod_{i=p+1}^{k} e^{r_i-2}\right) \frac{r_p-2}{2\,e^2}\, n_p + \frac{r_k-2}{2\,e^2}\, n_k \ . \quad (13)$$

2. *The Main Result*

According to Eq. (3), the terms $r_0, r_1, \ldots, r_k$ in the expression

$$\prod_{i=0}^{k} e^{r_i-2} \quad (14)$$

occurring on the right–hand side of (13) are fully determined by the degree r of the graph G. Thus, (14) depends solely on r and k.

According to Eqs. (4) and (6), the terms $n_0, n_1, \ldots, n_k$ in the expression

$$\sum_{p=0}^{k-1} \left(\prod_{i=p+1}^{k} e^{r_i-2}\right) \frac{r_p-2}{2\,e^2}\, n_p + \frac{r_k-2}{2\,e^2}\, n_k \quad (15)$$

occurring on the right–hand side of (13) are fully determined by the order n and degree r of the graph G and are, in addition, linearly proportional to the parameter n. Consequently, (15) depends solely on n, r, and k, and is linearly proportional to n.

Bearing the above in mind we arrive at:

Theorem 3. *The Estrada index of a regular graph G of order n and degree $r \geq 3$, and of its iterated line graphs are related in the following manner*

$$EE(L^k(G)) = a_k(r)\, EE(G) + b_k(r)\, n$$

where $a_k(r)$ and $b_k(r)$ are functions depending solely on the variable r and parameter k, $k \geq 1$.

3. *On the Functions $a_k(r)$ and $b_k(r)$*

From (8) we immediately see that

$$\begin{aligned} a_1(r) &= e^{r-2} \\ b_1(r) &= \frac{r-2}{2\,e^2}\,. \end{aligned}$$

Using the relations (2), from (10) we obtain

$$\begin{aligned} a_2(r) &= e^{3(r-2)} \\ b_2(r) &= \frac{r-2}{2\,e^2}\left[e^{2(r-2)} + r\right]\,. \end{aligned}$$

Analogously, from (11) there follows

$$\begin{aligned} a_3(r) &= e^{7(r-2)} \\ b_3(r) &= \frac{r-2}{2\,e^2}\left[e^{6(r-2)} + r\,e^{4(r-2)} + 2r(r-1)\right]\,. \end{aligned}$$

Using the relation (3), the general form of the function $a_k(r)$ is easy to find. For $k \geq 1$, from (14),

$$a_k(r) = \prod_{i=0}^{k-1} e^{r_i - 2} = \prod_{i=0}^{k-1} e^{\left(2^i\,r - 2^{i+1} + 2\right) - 2} = \prod_{i=0}^{k-1} e^{(r-2)\,2^i} = e^{\sum\limits_{i=0}^{k-1} (r-2)\,2^i}\,,$$

which finally yields

$$a_k(r) = e^{(r-2)(2^k - 1)}\,. \tag{16}$$

The function $b_k(r)$ cannot be transformed into a similarly simple form. For $k = 1,2,3$, expressions for $b_k(r)$ are given above. Therefore, in what follows we assume that $k \geq 4$. By combining (6) and (15) we get

$$b_k(r) = \sum_{p=0}^{k-2} \left(\prod_{i=p+1}^{k-1} e^{r_i - 2} \right) \frac{r_p - 2}{2\,e^2}\,\gamma_p + \frac{r_{k-1} - 2}{2\,e^2}\,\gamma_{k-1} \ ,$$

which after a lengthy calculation, taking into account (5), becomes

$$\begin{aligned} b_k(r) \ = \ & \frac{r-2}{2\,e^2}\, e^{(r-2)\,2^k} \ \times \\ & \times \ \left[e^{-2(r-2)} + r\,e^{-4(r-2)} + \sum_{p=2}^{k-2} r\,e^{-(r-2)2^{p+1}}\, 2^{p-1} \prod_{i=1}^{p-1} \left(2^{i-1}\,r - 2^i + 1 \right) \right] \\ & + \ \frac{r(r-2)}{8\,e^2}\, 2^k \prod_{i=1}^{k-2} \left(2^{i-1}\,r - 2^i + 1 \right) \ . \end{aligned}$$

Both $a_k(r)$ and $b_k(r)$ are rapidly increasing functions of both r and k. From Eq. (16) it is immediately seen that for $k \to \infty$,

$$a_k(r) = O\left(e^{(r-2)\,2^k} \right)$$

i.e., that for all values of r , $0 < r < \infty$,

$$0 < \lim_{k\to\infty} \frac{a_k(r)}{e^{(r-2)\,2^k}} < \infty \ .$$

We now show that the asymptotic behavior of the function $b_k(r)$ is analogous, namely that

$$b_k(r) = O\left(e^{(r-2)\,2^k} \right) \ . \tag{17}$$

In view of Eq. (4), the term $[(r_k - 2)/(2\,e^2)]\, n_k$, occurring in Eq. (9), can be written as $K\,d_k$, where

$$K = \frac{1}{4}\, nr(r-2)\, e^{-2} = const$$

and

$$d_k := 2^k \prod_{i=1}^{k-1} \left[2^{i-1}\,(r-2) + 1 \right] \ . \tag{18}$$

Then

$$EE(L^{k+1}(G)) = e^{r_k-2}\, e^{r_{k-1}-2} \cdots e^{r_2-2}\, EE(L^2(G)) + c_k \ ,$$

where

$$\begin{aligned} c_k &:= K \sum_{p=3}^{k} e^{r_k-2} \cdots e^{r_p-2}\, d_{p-1} + K\, d_k \\ &= K\, e^{(r-2)\,2^{k+1}} \sum_{p=3}^{k} e^{-(r-2)\,2^p}\, 2^{p-1} \prod_{i=1}^{p-2} \Big[2^{i-1}\,(r-2)+1\Big] + K\, d_k \ . \end{aligned}$$

The sequence $\{f_k\}$, defined via

$$f_k := \sum_{p=3}^{k} e^{-(r-2)\,2^p}\, 2^{p-1} \prod_{i=1}^{p-2} \Big[2^{i-1}\,(r-2)+1\Big]$$

is bounded from above. To see this note that for $r > 2$ and $i \geq 1$,

$$(r-2)\,2^{i-1} + 1 \leq (r-2)\,2^{i-1} + (r-2)\,2^{i-1} = (r-2)\,2^i$$

from which

$$\begin{aligned} \prod_{i=1}^{p-2} \Big[(r-2)\,2^{i-1}+1\Big] &\leq \prod_{i=1}^{p-2} (r-2)\,2^i = (r-2)^{p-2}\, 2^{1+2+\cdots+(p-2)} \\ &= (r-2)^{p-2}\, 2^{(p-1)(p-2)/2} \end{aligned}$$

from which

$$\begin{aligned} f_k &= \sum_{p=3}^{k} e^{-(r-2)\,2^p}\, 2^{p-1} \prod_{i=1}^{p-2} \Big[2^{i-1}\,(r-2)+1\Big] \\ &leq \sum_{p=3}^{k} e^{-(r-2)\,2^p}\, 2^{p-1}\, (r-2)^{p-2}\, 2^{(p-1)(p-2)/2} \\ &= \sum_{p=3}^{k} \frac{(r-2)^{p-2}\, 2^{p(p-1)/2}}{e^{(r-2)\,2^p}} < \sum_{p=3}^{+\infty} \frac{(r-2)^{p-2}\, 2^{p(p-1)/2}}{e^{(r-2)\,2^p}} \ . \end{aligned}$$

The latter series converges by D'Alembert's criterion. Indeed, let

$$g_p := \frac{(r-2)^{p-2}\, 2^{p(p-1)/2}}{e^{(r-2)\, 2^p}} \ .$$

Then the quotient

$$\frac{g_{p+1}}{g_p} = \frac{(r-2)\, 2^p}{e^{(r-2)\, 2^p}}$$

evidently tends to zero for $p \to \infty$.

Since the series $\{g_p\}$ converges, the sequence $\{f_k\}$ is bounded. Therefore, for $k \to \infty$,

$$c_k - K\, d_k = K\, e^{(r-2)\, 2^{k+1}} f_k = O\left(e^{(r-2)\, 2^{k+1}}\right) \ .$$

Using the above specified notation,

$$b_{k+1}(r) = h_k + K\, e^{(r-2)\, 2^{k+1}} f_k + K\, d_k \tag{19}$$

where

$$h_k := e^{(r-2)(2^{k+1}-4)} \left[\frac{r-2}{2\, e^2}\, e^{2(r-2)} + \frac{r(r-2)}{2\, e^2}\right] \ .$$

For $k \to \infty$,

$$h_k = O\left(e^{(r-2)\, 2^{k+1}}\right)$$

and, consequently,

$$h_k + K\, e^{(r-2)\, 2^{k+1}} f_k = O\left(e^{(r-2)\, 2^{k+1}}\right) \ . \tag{20}$$

Let p be the smallest integer for which $r-2 \le 2^p$ holds. Then from (18) there follows

$$d_k < 2^k \prod_{i=1}^{k-1} \left[2^i\, (r-2)\right] \le 2^k \prod_{i=1}^{k-1} \left[2^i\, 2^p\right] = 2^{p(k-1)+k(k+1)/2}$$

for $r > 2$, which implies

$$\lim_{k\to\infty} \frac{d_k}{e^{(r-2)\, 2^{k+1}}} = 0 \ .$$

Therefore, for $k \to \infty$,

$$d_k = o\left(e^{(r-2)\, 2^{k+1}}\right) \quad \Rightarrow \quad d_k = O\left(e^{(r-2)\, 2^{k+1}}\right) \ . \tag{21}$$

The property (17) of the function $b_k(r)$ follows now when the relations (20) and (21) are combined with (19).

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REFERENCES

[1] F. B u c k l e y, *Iterated line graphs*, Congr. Numer. **33** (1981) 390–394.

[2] F. B u c k l e y, *The size of iterated line graphs*, Graph Theory Notes New York **25** (1993) 33–36.

[3] D. C v e t k o v i ć, M. D o o b, H. S a c h s, *Spectra of Graphs – Theory and Application*, Academic Press, New York, 1980; 2nd revised ed.: Barth, Heidelberg, 1995.

[4] J. A. d e l a P e ñ a, I. G u t m a n, J. R a d a, *Estimating the Estrada index*, Lin. Algebra Appl. **427** (2007), 70–76.

[5] E. E s t r a d a, *Characterization of 3D molecular structure*, Chem. Phys. Lett. **319** (2000) 713–718.

[6] E. E s t r a d a, *Characterization of the folding degree of proteins*, Bioinformatics **18** (2002) 697–704.

[7] E. E s t r a d a, *Characterization of the amino acid contribution to the folding degree of proteins*, Proteins **54** (2004) 727–737.

[8] E. E s t r a d a, *Topological structural classes of complex networks*, Phys. Rev. **E 75** (2007) 016103–1–12.

[9] E. E s t r a d a, J. A. R o d r í g u e z – Ve l á z q u e z, *Subgraph centrality in complex networks*, Phys. Rev. **E 71** (2005) 056103–1–9.

[10] E. E s t r a d a, J. A. R o d r í g u e z – V e l á z q u e z, *Spectral measures of bipartivity in complex networks*, Phys. Rev. **E 72** (2005) 046105–1–6.

[11] I. G u t m a n, *Lower bounds for Estrada index*, Publ. Inst. Math. (Beograd), in press

[12] I. G u t m a n, A. G r a o v a c, *Estrada index of cycles and paths*, Chem. Phys. Lett. **436** (2007), 294–296.

[13] H. S a c h s, *Über Teiler, Faktoren und charakteristische Polynome von Graphen. Teil II*, Wiss. Z. TH Ilmenau **13** (1967) 405–412.

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