MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **73** (2015) 133-148

ISSN 0340 - 6253

Coulson-Type Integral Formulas for the Estrada Index of Graphs and the Skew Estrada Index of Oriented Graphs

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(Received March 31, 2014)

Abstract

The energy of graphs and skew energy of oriented graphs have been studied extensively in recent years. The Estrada index, an invariant of graphs, which is similar to the energy, has also received much attention nowadays. Motivated by these three graph invariants, in this paper, we introduce a new one, the skew Estrada index of oriented graphs. For an oriented graph G^σ with n vertices, its skew Estrada index is defined as $EE_s(G^\sigma) = \sum_{k=1}^{n} e^{i\lambda_k}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G^σ. A well-known result on the energy of graphs is the Coulson integral formula which was given by Coulson in 1940. Our main results in this paper are some integral formulas for the Estrada index of graphs and the skew Estrada index of oriented graphs, which are counterparts of the Coulson integral formula for the energy of graphs.

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1 Introduction

All graphs considered in this paper are finite and simple. Let G be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and $A(G) = [a_{ij}]$ be the adjacency matrix of G, where $a_{ij} = 1$ if the vertices v_i and v_j are adjacent, and $a_{ij} = 0$ otherwise. The *eigenvalues* of the adjacency matrix $A(G)$ are said to be the eigenvalues of G. We denote the eigenvalues of G by $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ in non-increasing order. Since $A(G)$ is symmetric, all eigenvalues of $A(G)$ are real. The *energy* of G was defined in the 1970s by

$$E(G) = \sum_{k=1}^{n} |\lambda_k|,$$

which is derived from the total π-electron energy [22]. Graph energy has been studied extensively by many mathematicians and chemists, and there have been many results obtained on this invariant of graphs (see [18]).

Let G^σ be an *oriented graph* of a graph G with an orientation σ. Then G is usually called the *underlying graph* of G^σ. Throughout this paper, we assume that G^σ does not have loops and multiple arcs. If the vertex set of G^σ is $\{v_1, v_2, \ldots, v_n\}$, then the *skew-adjacency matrix* of G^σ is defined as $S(G^\sigma) = (s_{ij})$, where $s_{ij} = 1$ and $s_{ji} = -1$ if there is an arc from v_i to v_j in G^σ, otherwise $s_{ij} = s_{ji} = 0$. Adiga *et al.* [1] introduced the concept of the *skew energy* of G^σ as

$$E_s(G^\sigma) = \sum_{k=1}^{n} |\lambda_k|,$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all eigenvalues of the skew-adjacency matrix $S(G^\sigma)$. Since $S(G^\sigma)$ is a skew-symmetric matrix, the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $S(G^\sigma)$ are pure imaginary and occur in complex conjugate pairs. Most of the results on the skew energy are collected in the survey [17].

There is an important integral formula called *Coulson integral formula* in the theory of graph energy which makes it possible to calculate the energy of a graph without knowing its spectrum. That is, for a graph G,

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \left[n - \frac{ix\phi'(G, ix)}{\phi(G, ix)} \right] dx,$$

where $\phi(G,x)$ is the characteristic polynomial of $A(G)$ (called the *characteristic polynomial* of G). This formula was obtained by Coulson [3], and has many applications in the theory of graph energy (see [18]).

Similar to the Coulson formula for the energy of undirected graph, Adiga *et al.* [1] deduced an integral formula for the skew energy of an oriented graph. That is, for an oriented graph G^σ on n vertices,

$$E_s(G^\sigma) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\left[n + x\frac{\phi'(G^\sigma,-x)}{\phi(G^\sigma,-x)}\right]dx,$$

where $\phi(G^\sigma,x)$ is the *skew-characteristic polynomial* of G^σ.

In algebraic and chemical theory, there are many other graph-spectrum-based invariants. Among them, the *Estrada index*, introduced by Estrada [8], is defined as

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

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all eigenvalues of the adjacency matrix $A(G)$. Since its introduction in 2000 as a molecular structure-descriptor, Estrada index has found various applications in many fields, such as biology, quantum chemistry and complex networks [8, 9, 10, 11, 12, 13]. In addition, this graph invariant has also received much attention from pure mathematicians for theoretical research. We refer the reader to the references [5, 6, 7, 15, 19, 23]. For a recent survey on Estrada index, we refer to [16].

Motivated by the Estrada index of graphs and the skew energy of oriented graphs, here we introduce the *skew Estrada index* as follows.

Definition 1.1 *For an oriented graph G^σ with n vertices, the skew Estrada index of G^σ, denoted by $EE_s(G^\sigma)$ is defined as*

$$EE_s(G^\sigma) = \sum_{k=1}^{n} e^{i\lambda_k},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all the eigenvalues of the skew-adjacency matrix $S(G^\sigma)$.

Inspired by the Coulson integral formula for the energy of graphs and the integral formula for the skew energy of oriented graphs, in this paper, we will give some integral formulas for the Estrada index of graphs and the skew Estrada index of oriented graphs, at a rigorous mathematical level.

2 Preliminaries

We first introduce some basic concepts and results of complex analysis which will be used in our paper later. A *complex number* is an expression of the form $z = x + iy = r(\cos\theta + i\sin\theta) = re^{i\theta}$, where $x,\ y,\ r\ (>0),\ \theta$ are real numbers, and $i = \sqrt{-1}$ is the imaginary unit. The correspondence

$$z = x + iy \longleftrightarrow (x, y)$$

is a one-to-one correspondence between complex numbers which are in the complex plane $\mathbb{C}$ and points (or vectors) in the Euclidean plane $\mathbb{R}^2$.

The *Cauchy principal value P.V.* of the integral $P.V. \int\limits_{-\infty}^{+\infty} f(x)dx$ of a function $f(x)$ over the interval $(-\infty, +\infty)$ means $\lim\limits_{M\to+\infty} \int\limits_{-M}^{M} f(x)dx$. In the case that $f(x)$ has real singularities $a_1 < a_2 < \cdots < a_s$, the *Cauchy principal value P.V.* of the integral $P.V. \int\limits_{-\infty}^{+\infty} f(x)dx$ will stand for

$$\lim_{\substack{M\to+\infty \\ \varepsilon_j\to 0 (j=1,\cdots,s)}} \left(\int_{-M}^{a_1-\varepsilon_1} f(x)dx + \sum_{j=1}^{s-1} \int_{a_j+\varepsilon_j}^{a_{j+1}-\varepsilon_{j+1}} f(x)dx + \int_{a_s+\varepsilon_s}^{M} f(x)dx \right).$$

The following two results in complex analysis are well known (see [14]).

Lemma 2.1 (Cauchy's Theorem) *Let D be a bounded domain with piecewise smooth boundary. If $f(z)$ is analytic on D that extends smoothly to ∂D, then*

$$\int_{\partial D} f(z)dz = 0.$$

Lemma 2.2 (Cauchy Integral Formula) *Let D be a bounded domain with piecewise smooth boundary. If $f(z)$ is analytic on D, and $f(z)$ extends smoothly to the boundary of D, then*

$$f(z) = \frac{1}{2\pi i} \int_{\partial D} \frac{f(w)}{w - z} dw, \ \ z \in D.$$

Lemma 2.3 (Jordan's Lemma) *Let Γ_R be the semicircular contour $z(\theta) = Re^{i\theta}$, $0 \le \theta \le \pi$, in the upper half-plane, where R is a positive real number. If $g(z)$ is a continuous* *function on the semicircular contour* Γ_R *for all large* R *such that*

$$\lim_{R\to+\infty}\max_{\theta\in[0,\pi]}|g(Re^{i\theta})|=0,$$

then

$$\lim_{R\to+\infty}\int_{\Gamma_R} g(z)e^{imz}dz=0\ (m>0).$$

The following lemma can be viewed as a deformation of the famous Jordan's Lemma (see [14]).

Lemma 2.4 *Let* Γ_R *be the semicircular contour* $z(\theta)=Re^{i\theta}$, $\frac{\pi}{2}\le\theta\le\frac{3\pi}{2}$, *in the left half-plane, where* R *is a positive real number. If* $g(z)$ *is a continuous function on the semicircular contour* Γ_R *for all large* R *such that*

$$\lim_{R\to+\infty}\max_{\theta\in[\frac{\pi}{2},\frac{3\pi}{2}]}|g(Re^{i\theta})|=0,$$

then

$$\lim_{R\to+\infty}\int_{\Gamma_R} g(z)e^{mz}dz=0\ (m>0).$$

Proof. For any $\varepsilon>0$, there exists $R_0=R_0(\varepsilon)>0$, such that $|g(z)|<\varepsilon$, $z\in\Gamma_R$, for $R>R_0$. Therefore, from the facts $|g(Re^{i\theta})|<\varepsilon$, $|Re^{i\theta}i|=R$, and

$$|e^{mRe^{i\theta}}|=|e^{mR\cos\theta+imR\sin\theta}|=e^{mR\cos\theta},$$

we have

$$\begin{aligned}\left|\int_{\Gamma_R} g(z)e^{mz}dz\right| &= \left|\int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} g(Re^{i\theta})e^{mRe^{i\theta}}Re^{i\theta}id\theta\right| \\ &\le R\varepsilon\int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} e^{mR\cos\theta}d\theta \\ &= R\varepsilon\int_0^{\pi} e^{-mR\sin t}dt,\end{aligned}$$

where $t=\theta-\frac{\pi}{2}$.

By Jordan's Inequality $\frac{2\theta}{\pi}\le\sin\theta\le\theta\ (0\le\theta\le\frac{\pi}{2})$, we get

$$
\begin{aligned}
\left|\int_{\Gamma_R} g(z)e^{mz}dz\right| &\leq 2R\varepsilon \int_0^{\frac{\pi}{2}} e^{-mR\sin t}dt \\
&\leq 2R\varepsilon \int_0^{\frac{\pi}{2}} e^{-\frac{2mRt}{\pi}}dt \\
&= 2R\varepsilon \left[-\frac{e^{-\frac{2mR}{\pi}t}}{\frac{2mR}{\pi}}\right]\Bigg|_{t=0}^{t=\frac{\pi}{2}} \\
&= \frac{\pi\varepsilon}{m}(1-e^{-mR}) < \frac{\pi\varepsilon}{m}.
\end{aligned}
$$

This completes the proof. ∎

We also need the following lemma which is simple and we omit the proof here.

Lemma 2.5 *Let S_r be the arc $z(\theta) = a_0 + re^{i\theta}$, $\theta_1 \leq \theta \leq \theta_2$, where $r > 0$ is a real number. If $g(z)$ is a continuous function on the arc S_r for all small r such that*

$$
\lim_{r\to 0^+} \max_{\theta\in[\theta_1,\theta_2]} |re^{i\theta}g(a_0+re^{i\theta}) - \lambda| = 0,
$$

then

$$
\lim_{r\to 0^+} \int_{S_r} g(z)dz = i(\theta_2-\theta_1)\lambda.
$$

3 Integral formulas for the Estrada index of graphs

Let Γ be a simple, positively (i.e., counter-clockwisely) oriented and piecewise smooth contour in the complex plane, and z_0 a complex number in the interior of Γ. Then by Cauchy Integral Formula, we have

$$
e^z = \frac{1}{2\pi i}\int_\Gamma \frac{e^w}{w-z}dw.
$$

Let $\phi(G,x)$ be the characteristic polynomial of G, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G,x)$. Then

$$
\phi(G,x) = \prod_{k=1}^{n}(x-\lambda_k).
$$

Consequently, by a simple differentiation, we have

$$
\begin{aligned}
\phi'(G,x) =& (x-\lambda_2)(x-\lambda_3)\cdots(x-\lambda_n) + (x-\lambda_1)(x-\lambda_3)\cdots(x-\lambda_n) \\
&+ \cdots + (x-\lambda_1)(x-\lambda_2)\cdots(x-\lambda_{n-1}),
\end{aligned}
$$

which gives

$$\frac{\phi'(G,x)}{\phi(G,x)} = \sum_{k=1}^{n} \frac{1}{x-\lambda_k}.$$

Therefore, the Estrada index of G is

$$EE(G) = \sum_{k=1}^{n} e^{\lambda_k} = \frac{1}{2\pi i} \sum_{k=1}^{n} \int_{\Gamma} \frac{e^z}{z-\lambda_k} dz = \frac{1}{2\pi i} \int_{\Gamma} \frac{\phi'(G,z)}{\phi(G,z)} e^z dz, \qquad (3.1)$$

if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all in the interior of Γ.

With Lemma 2.4, we can obtain our first main result.

Theorem 3.1 *Let G be an n-vertex graph, $\phi(G,x)$ the characteristic polynomial of G, $\lambda_1, \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G,x)$, and M a positive real number such that $|\lambda_k| < M,\ k = 1, 2, \ldots, n$. Then the Estrada index of G can be given by the following integral formula*

$$EE(G) = \frac{1}{2\pi}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G, ix+M)}{\phi(G, ix+M)} e^{ix+M} dx.$$

Proof. Suppose that $\Gamma = \Gamma_R \cup L$ is a positively (i.e., counter-clockwisely) oriented piecewise smooth contour, where Γ_R is the semicircular contour $\{z(\theta) = Re^{i\theta},\ \frac{\pi}{2} \le \theta \le \frac{3\pi}{2},\ R > 0\}$, and L is the line $\{z = iy,\ -R \le y \le R\}$ (see Figure 1). Since $|\lambda_k| < M,\ k = 1, 2, \ldots, n$, $\lambda_1 - M, \lambda_2 - M, \ldots, \lambda_n - M$ are all in the left half-plane. If $R > |\lambda_k - M|,\ k = 1, 2, \ldots, n$, then the points $\lambda_1 - M, \lambda_2 - M, \ldots, \lambda_n - M$ are all in the interior of the contour Γ. Therefore, by Equality (3.1), we obtain

$$\begin{aligned}
EE(G) = \sum_{k=1}^{n} e^{\lambda_k} &= e^M \sum_{k=1}^{n} e^{\lambda_k - M} \\
&= \frac{e^M}{2\pi i} \sum_{k=1}^{n} \int_{\Gamma} \frac{e^z}{z-(\lambda_k - M)} dz \\
&= \frac{e^M}{2\pi i} \int_{\Gamma} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \\
&= \frac{e^M}{2\pi i} \left(\int_{L} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz + \int_{\Gamma_R} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \right).
\end{aligned}$$

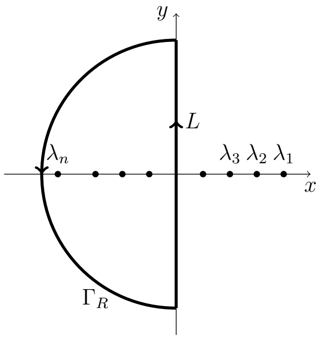

Figure 1: The contour Γ in Theorem 3.1.

Obviously,

$$\frac{\phi'(G, z+M)}{\phi(G, z+M)} \to 0, \text{ for } |z| \to +\infty.$$

By Lemma 2.4, we get

$$\int_{\Gamma_R} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \to 0, \text{ for } |z| \to +\infty.$$

Since the value of the following integral

$$\frac{e^M}{2\pi i} \int_{\Gamma} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \tag{3.2}$$

is independent of the actual form of the contour Γ (provided that all the zeros of $\phi(G, z+M)$ lie in the interior of Γ), we may choose R large enough and obtain

$$\begin{aligned} EE(G) &= \lim_{R\to+\infty} \frac{e^M}{2\pi i} \int_{\Gamma} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \\ &= \lim_{R\to+\infty} \frac{e^M}{2\pi i} \left(\int_L \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz + \int_{\Gamma_R} \frac{\phi'(G, z+M)}{\phi(G, z+M)} e^z dz \right) \\ &= \frac{e^M}{2\pi i}\, P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G, iy+M)}{\phi(G, iy+M)} e^{iy} i dy \\ &= \frac{1}{2\pi}\, P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G, ix+M)}{\phi(G, ix+M)} e^{ix+M} dx. \end{aligned}$$

This completes the proof. ∎

For a graph G, it is clear that $|\lambda_k| \le \lambda_1$, $k = 1, 2, \ldots, n$. Replacing M ($> \lambda_1$) in Theorem 3.1 with λ_1, we can obtain another integral formula for the Estrada index of G.

Theorem 3.2 *Let G be a connected n-vertex graph, $\phi(G,x)$ the characteristic polynomial of G, and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ the roots of $\phi(G,x)$. Then the Estrada index of G can be given by the following integral formula*

$$EE(G) = \frac{1}{2\pi}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G, ix+\lambda_1)}{\phi(G, ix+\lambda_1)} e^{ix+\lambda_1} dx - \frac{e^{\lambda_1}}{2}.$$

Proof. Since G is a connected graph, by Perron-Frobenius Theorem (see [2]), the multiplicity of λ_1 is 1. This implies that $\lambda_k - \lambda_1 < 0,\ k = 2, 3, \ldots, n$.

Suppose that $\Gamma = \Gamma_R \cup L_1 \cup S_r \cup L_2$ is a positively (i.e., counter-clockwisely) oriented piecewise smooth contour, where $R > |\lambda_n - \lambda_1|$, $0 < r < |\lambda_2 - \lambda_1|$, Γ_R is the semicircular contour $\{z(\theta) = Re^{i\theta},\ \frac{\pi}{2} \leq \theta \leq \frac{3\pi}{2}\}$, L_1 is the line $\{z = iy,\ -R \leq y \leq -r\}$, S_r is the the semicircular contour $\{z(\theta) = re^{i\theta},\ \frac{\pi}{2} \leq \theta \leq \frac{3\pi}{2}\}$, and L_2 is the line $\{z = iy,\ r \leq y \leq R\}$.

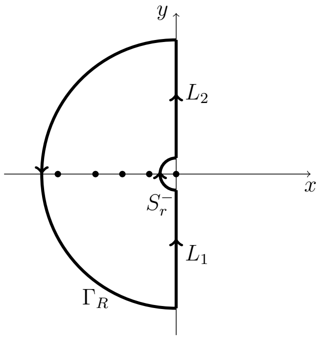

Figure 2: The contour Γ in Theorem 3.2.

Then the points $\lambda_2 - \lambda_1, \lambda_2 - \lambda_1, \ldots, \lambda_n - \lambda_1$ are all in the interior of the contour Γ. Therefore, we have

$$\begin{aligned} EE(G) = \sum_{k=1}^{n} e^{\lambda_k} &= e^{\lambda_1} + e^{\lambda_1} \sum_{k=2}^{n} e^{\lambda_k - \lambda_1} = e^{\lambda_1} + \frac{e^{\lambda_1}}{2\pi i} \sum_{k=2}^{n} \int_{\Gamma} \frac{e^z}{z - (\lambda_k - \lambda_1)} dz \\ &= e^{\lambda_1} + \frac{e^{\lambda_1}}{2\pi i} \int_{\Gamma} \frac{\phi'(G, z+\lambda_1)}{\phi(G, z+\lambda_1)} e^z dz \\ &= e^{\lambda_1} + \frac{e^{\lambda_1}}{2\pi i} \left(\int_{L_1} \frac{\phi'(G, z+\lambda_1)}{\phi(G, z+\lambda_1)} e^z dz + \int_{S_r^-} \frac{\phi'(G, z+\lambda_1)}{\phi(G, z+\lambda_1)} e^z dz \right. \\ &\left. + \int_{L_2} \frac{\phi'(G, z+\lambda_1)}{\phi(G, z+\lambda_1)} e^z dz + \int_{\Gamma_R} \frac{\phi'(G, z+\lambda_1)}{\phi(G, z+\lambda_1)} e^z dz \right), \end{aligned}$$

where S_r^- is the same curve as S_r but has clockwise orientation.

Since

$$\begin{aligned}\lim_{r\to 0^+} z\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z &= \lim_{r\to 0^+} z\sum_{k=1}^{n}\frac{e^z}{z-(\lambda_k-\lambda_1)}\\ &= \lim_{r\to 0^+}\left[1+\sum_{k=2}^{n}\frac{z}{z-(\lambda_k-\lambda_1)}\right]e^z = 1\end{aligned}$$

holds uniformly on the arc S_r, it follows from Lemma 2.5 that

$$\lim_{r\to 0^+}\int_{S_r^-}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz = -\lim_{r\to 0^+}\int_{S_r}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz = -i\pi.$$

By Lemma 2.4, we get

$$\int_{\Gamma_R}\frac{\phi'(G,z+M)}{\phi(G,z+M)}e^z dz \to 0, \text{ for } |z|\to +\infty.$$

Since the value of the following integral

$$\frac{e^M}{2\pi i}\int_{\Gamma}\frac{\phi'(G,z+M)}{\phi(G,z+M)}e^z dz \tag{3.3}$$

is independent of the actual form of the contour Γ, we obtain that

$$\begin{aligned}EE(G) &= e^{\lambda_1}+\frac{e^{\lambda_1}}{2\pi i}\lim_{\substack{R\to+\infty\\ r\to 0^+}}\Big(\int_{L_1}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz+\int_{S_r^-}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz\\ &\quad +\int_{L_2}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz+\int_{\Gamma_R}\frac{\phi'(G,z+\lambda_1)}{\phi(G,z+\lambda_1)}e^z dz\Big)\\ &= e^{\lambda_1}+\frac{e^{\lambda_1}}{2\pi i}\Big(\int_{-\infty}^{0}\frac{\phi'(G,iy+\lambda_1)}{\phi(G,iy+\lambda_1)}e^{iy}idy - i\pi + \int_0^{+\infty}\frac{\phi'(G,iy+\lambda_1)}{\phi(G,iy+\lambda_1)}e^{iy}idy + 0\Big)\\ &= \frac{1}{2\pi}\ P.V.\int_{-\infty}^{+\infty}\frac{\phi'(G,ix+\lambda_1)}{\phi(G,ix+\lambda_1)}e^{ix+\lambda_1}dx - \frac{e^{\lambda_1}}{2}.\end{aligned}$$

This completes the proof. ∎

4 Integral formula for the Estrada index of polynomials

Mateljević, Božin and Gutman [20] introduced the concept of the energy of a polynomial. Later, Shao, Gong and Gutman [21] gave an integral formula for it. As a generalization of the Estrada index of a graph, the Estrada index of a complex polynomial can be introduced as follows.

Definition 4.1 *Let*

$$\phi(z) = \sum_{k=0}^{n} a_k z^{n-k} = a_0 \prod_{k=1}^{n} (z - z_k)$$

be a complex polynomial of degree n. Then its (complex) Estrada index $EE(\phi)$ is defined as

$$EE(\phi) = \sum_{k=1}^{n} e^{z_k}.$$

By a similar argument in the proof of Theorem 3.1, we can obtain the following more general result.

Theorem 4.1 *Let $\phi(z)$ be a monic polynomial of degree n, $z_1, z_2, \ldots, z_n$ the roots of $\phi(z)$, and M a positive real number such that $|z_k| < M,\ k = 1, 2, \ldots, n$. Then the Estrada index of $\phi(z)$ can be given by the following integral formula*

$$EE(\phi) = \frac{1}{2\pi}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(ix+M)}{\phi(ix+M)} e^{ix+M} dx.$$

5 Integral formulas for the skew Estrada index of oriented graphs

Let $\phi(G^\sigma, x)$ be the skew-characteristic polynomial of G^σ, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G^\sigma, x)$. Then the skew Estrada index of G^σ is

$$EE_s(G^\sigma) = \sum_{k=1}^{n} e^{i\lambda_k} = \frac{1}{2\pi i} \sum_{k=1}^{n} \oint_\Gamma \frac{e^{iz}}{z - \lambda_k} dz = \frac{1}{2\pi i} \oint_\Gamma \frac{\phi'(G^\sigma, z)}{\phi(G^\sigma, z)} e^{iz} dz, \tag{5.4}$$

if $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all in the interior of Γ.

With Lemma 2.3, we can obtain our the following result.

Theorem 5.1 *Let G^σ be an n-vertex oriented graph, $\phi(G^\sigma, x)$ the skew-characteristic polynomial of G^σ, $\lambda_1,\ \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G^\sigma, x)$, and M a positive real number such that $|\lambda_k| < M,\ k = 1, 2, \ldots, n$. Then the skew Estrada index of G^σ can be given by the following integral formula*

$$EE_s(G^\sigma) = \frac{1}{2\pi i}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G^\sigma, x - iM)}{\phi(G^\sigma, x - iM)} e^{ix+M} dx.$$

Proof. Suppose that $\Gamma = \Gamma_R \cup L$ is a positively (i.e., counter-clockwisely) oriented piecewise smooth contour, where Γ_R is the semicircular contour $\{z(\theta) = Re^{i\theta},\ 0 \leq \theta \leq \pi,\ R > 0\}$, and L is the line $\{z = x,\ \ -R \leq x \leq R\}$ (see Figure 3). Since $|\lambda_k| < M,\ k = 1, 2, \dots, n$, $\lambda_1 + iM, \lambda_2 + iM, \dots, \lambda_n + iM$ are all in the upper half-plane. If $R > |\lambda_k + iM|,\ k = 1, 2, \dots, n$, then the points $\lambda_1 + iM, \lambda_2 + iM, \dots, \lambda_n + iM$ are all in the interior of the contour Γ. Therefore, by equality (5.4), we obtain

$$\begin{aligned} EE_s(G^\sigma) &= \sum_{k=1}^{n} e^{i\lambda_k} = e^M \sum_{k=1}^{n} e^{i(\lambda_k + iM)} = \frac{e^M}{2\pi i} \sum_{k=1}^{n} \oint_\Gamma \frac{e^{iz}}{z - (\lambda_k + iM)} dz \\ &= \frac{e^M}{2\pi i} \oint_\Gamma \frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} e^{iz} dz = \frac{e^M}{2\pi i} \left(\int_L \frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} e^{iz} dz \right. \\ &\left. + \int_{\Gamma_R} \frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} e^{iz} dz \right). \end{aligned}$$

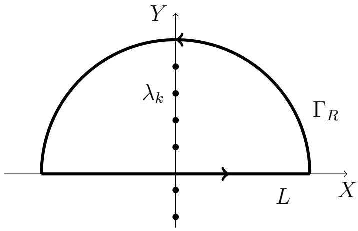

Figure 3: The contour Γ in Theorem 5.1.

Obviously,

$$\frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} \to 0, \text{ for } |z| \to +\infty.$$

By Lemma 2.4, we get

$$\int_{\Gamma_R} \frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} e^{iz} dz \to 0, \text{ for } |z| \to +\infty.$$

Since the value of the following integral

$$\frac{e^M}{2\pi i} \oint_\Gamma \frac{\phi'(G^\sigma, z - iM)}{\phi(G^\sigma, z - iM)} e^{iz} dz \tag{5.5}$$

is independent of the actual form of the contour Γ (provided that all the zeros of $\phi(G^\sigma, z-$

iM) lie in the interior of Γ), we may choose R large enough and obtain

$$\begin{aligned} EE_s(G^\sigma) &= \lim_{R\to+\infty} \frac{e^M}{2\pi i} \oint_\Gamma \frac{\phi'(G^\sigma, z-iM)}{\phi(G^\sigma, z-iM)} e^{iz} dz \\ &= \lim_{R\to+\infty} \frac{e^M}{2\pi i} \left(\int_L \frac{\phi'(G^\sigma, z-iM)}{\phi(G^\sigma, z-iM)} e^{iz} dz + \int_{\Gamma_R} \frac{\phi'(G^\sigma, z-iM)}{\phi(G^\sigma, z-iM)} e^{iz} dz \right) \\ &= \frac{e^M}{2\pi i}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G^\sigma, x-iM)}{\phi(G^\sigma, x-iM)} e^{ix} dx = \frac{1}{2\pi i}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G^\sigma, x-iM)}{\phi(G^\sigma, x-iM)} e^{ix+M} dx. \end{aligned}$$

This completes the proof. ∎

Let G^σ be an n-vertex oriented graph, $\phi(G^\sigma, x)$ the skew-characteristic polynomial of G^σ, $\lambda_1, \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G^\sigma, x)$. Suppose that Im $\lambda_1 \geq$ Im $\lambda_2 \geq \cdots \geq$ Im λ_n, and the multiplicity of λ_n is t. Replacing M ($< |\lambda_n|$) in Theorem 5.1 with $|\lambda_n|$, we can obtain another integral formula for the skew Estrada index of G^σ.

Theorem 5.2 *Let G^σ be an n-vertex oriented graph, $\phi(G^\sigma, x)$ the skew-characteristic polynomial of G^σ, $\lambda_1, \lambda_2, \ldots, \lambda_n$ the roots of $\phi(G^\sigma, x)$. Suppose that Im $\lambda_1 \geq$ Im $\lambda_2 \geq \cdots \geq$ Im λ_n, and the multiplicity of λ_n is t. Then the skew Estrada index of G^σ can be given by the following integral formula*

$$EE_s(G) = \frac{1}{2\pi i}\ P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G^\sigma, x-i|\lambda_n|)}{\phi(G^\sigma, x-i|\lambda_n|)} e^{ix+|\lambda_n|} dx - \frac{te^{|\lambda_n|}}{2}.$$

Proof. Suppose that $\Gamma = \Gamma_R \cup L_1 \cup S_r \cup L_2$ is a positively (i.e., counter-clockwisely) oriented piecewise smooth contour, where $R > |\lambda_n|$, $0 < r < |\lambda_n| - |\lambda_{n-1}|$, Γ_R is the semicircular contour $\{z(\theta) = Re^{i\theta},\ 0 \leq \theta \leq \pi\}$, L_1 is the line $\{z = x,\ -R \leq x \leq -r\}$, S_r is the the semicircular contour $\{z(\theta) = re^{i\theta},\ 0 \leq \theta \leq \pi\}$, and L_2 is the line $\{z = x,\ r \leq x \leq R\}$. Then the points $\lambda_k + i|\lambda_n|$ $(k = 1, 2, \ldots, n)$ are all in the interior of the contour Γ.

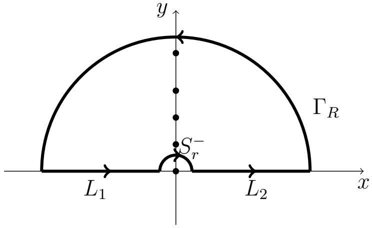

Figure 4: The contour Γ in Theorem 5.2.

Therefore, we have

$$
\begin{aligned}
EE_s(G) = \sum_{k=1}^{n} e^{i\lambda_k} &= te^{i\lambda_n} + \sum_{k=1}^{n-t} e^{i\lambda_k} = te^{i\lambda_n} + e^{|\lambda_n|}\sum_{k=1}^{n-t} e^{i(\lambda_k+i|\lambda_n|)} \\
&= te^{i\lambda_n} + \frac{e^{|\lambda_n|}}{2\pi i}\sum_{k=1}^{n-t}\oint_\Gamma \frac{e^{iz}}{z-(\lambda_k+i|\lambda_n|)}dz \\
&= te^{i\lambda_n} + \frac{e^{|\lambda_n|}}{2\pi i}\oint_\Gamma \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz \\
&= te^{i\lambda_n} + \frac{e^{|\lambda_n|}}{2\pi i}\Big(\int_{L_1} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz \\
&+ \int_{S_r^-} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz \\
&+ \int_{L_2} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz + \int_{\Gamma_R} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz\Big),
\end{aligned}
$$

where S_r^- is the same curve as S_r but has clockwise orientation.

Since

$$
\begin{aligned}
\lim_{r\to 0^+} z\frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz} &= \lim_{r\to 0^+} z\sum_{k=1}^{n}\frac{e^{iz}}{z-(\lambda_k+i|\lambda_n|)} \\
&= \lim_{r\to 0^+}\left[t + \sum_{k=1}^{n-t}\frac{z}{z-(\lambda_k+i|\lambda_n|)}\right]e^{iz} \\
&= t
\end{aligned}
$$

holds uniformly on the arc S_r, it follows from Lemma 2.5 that

$$
\lim_{r\to 0^+}\int_{S_r^-} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz = -\lim_{r\to 0^+}\int_{S_r} \frac{\phi'(G^\sigma, z-i|\lambda_n|)}{\phi(G^\sigma, z-i|\lambda_n|)}e^{iz}dz = -t\pi i.
$$

By Lemma 2.4, we get

$$
\int_{\Gamma_R} \frac{\phi'(G^\sigma, z-iM)}{\phi(G^\sigma, z-iM)}e^{iz}dz \to 0, \text{ for } |z| \to +\infty.
$$

Since the value of the following integral

$$
\frac{e^M}{2\pi i}\oint_\Gamma \frac{\phi'(G^\sigma, z-iM)}{\phi(G^\sigma, z-iM)}e^{iz}dz \tag{5.6}
$$

is independent of the actual form of the contour Γ, we obtain that

$$\begin{aligned}
EE_s(G) &= te^{i\lambda_n} + \frac{e^{|\lambda_n|}}{2\pi i} \lim_{\substack{R\to+\infty \\ r\to 0+}} \Big(\int_{L_1} \frac{\phi'(G^\sigma, z - i|\lambda_n|)}{\phi(G^\sigma, z - i|\lambda_n|)} e^{iz} dz + \int_{S_r^-} \frac{\phi'(G^\sigma, z - i|\lambda_n|)}{\phi(G^\sigma, z - i|\lambda_n|)} e^{iz} dz \\
&\quad + \int_{L_2} \frac{\phi'(G^\sigma, z - i|\lambda_n|)}{\phi(G^\sigma, z - i|\lambda_n|)} e^{iz} dz + \int_{\Gamma_R} \frac{\phi'(G^\sigma, z - i|\lambda_n|)}{\phi(G^\sigma, z - i|\lambda_n|)} e^{iz} dz \Big) \\
&= te^{i\lambda_n} + \frac{e^{|\lambda_n|}}{2\pi i} \Big(\int_{-\infty}^{0} \frac{\phi'(G^\sigma, x - i|\lambda_n|)}{\phi(G^\sigma, x - i|\lambda_n|)} e^{ix} dx - t\pi i \\
&\quad + \int_{0}^{+\infty} \frac{\phi'(G^\sigma, x - i|\lambda_n|)}{\phi(G^\sigma, x - i|\lambda_n|)} e^{ix} dx + 0 \Big) \\
&= \frac{1}{2\pi i} \, P.V. \int_{-\infty}^{+\infty} \frac{\phi'(G^\sigma, x - i|\lambda_n|)}{\phi(G^\sigma, x - i|\lambda_n|)} e^{ix + |\lambda_n|} dx - \frac{te^{|\lambda_n|}}{2}.
\end{aligned}$$

This completes the proof. ∎

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