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On the Energy of Trees

Jingyuan Zhang*, **Sen Qin**

School of Science, Hangzhou Dianzi University, Hangzhou 310018, P. R. China
jyzhang@hdu.edu.cn, qinsen0425@hdu.edu.cn

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Abstract

We use a polynomial $f(x) = \sum_{j=0}^{n_0}(-1)^j m(T,j)x^{n_0-j}$ for calculating the energy $E(T)$ of a tree T, where $m(T,j)$ and n_0 are the number of j-matchings and the maximal matching of T, respectively. To derive the exact expression of $E(T)$, we further consider a related polynomial $f(x)/d(x) = c_0x^m + c_1x^{m-1} + \cdots + c_m$, where $d(x)$ is the greatest common factor between $f(x)$ and its derivative $f'(x)$. Let $m_j = \lim_{p\to\infty} \frac{(f'(x_{j,p}))^2}{(f'(x_{j,p}))^2 - f(x_{j,p})f''(x_{j,p})}$, $\sqrt{x_j} = \lim_{p\to\infty}\sqrt{x_{j,p}}$, and $x_{j,p} = \sqrt[q]{\frac{c_{j,p}}{c_{j-1,p}}}$ with $q = 2^p$. We obtain the main result $E(T) = \sum_{j=1}^{m} 2m_j\sqrt{x_j}$, where $c_{j,p}$ for all $0 \le j \le m$ and $p \ge 0$ is recursively defined as follows: if $p = 0$, $c_{j,p} = c_j$; if $p \ge 1$, $c_{j,p} = c_{j,p-1}^2 + 2\sum_{k\ge1}(-1)^k c_{j-k,p-1}c_{j+k,p-1}$, and the summation is over "$j - k \ge 0$" and "$j + k \le m$". Additionally, we present a simple example to demonstrate the effectiveness of the new method.

1 Introduction

Let G be a simple graph with n vertices, and $\lambda_1, \ldots, \lambda_n$ its eigenvalues. Note that λ_j for each $1 \le j \le n$ is a zero of the characteristic polynomial $\phi(G,x) = \mathtt{det}(xI - A(G)) = x^n + a_1x^{n-1} + \cdots + a_n$, where $A(G)$ is the adjacency matrix of G. As well known [1],

*corresponding author

the graph energy $E(G)$ of G is defined as $E(G) = \sum_{j=1}^{n} |\lambda_j|$. It was introduced by Gutman in 1970s [2], and used as an approximation of the total π-electron energy [3]. In the last decade, research on graph energy, including bounds [4–12], hyperenergetic graphs [2, 13, 14], and equienergetic graphs [15, 16], to name just a few, has not only been a very popular topic, but resulted in over one hundred published papers [1]. The following formula is well known

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{1}{x^2} \log |x^n \phi(G, i/x)| \, \mathtt{dx}$$

where $i = \sqrt{-1}$. Furthermore, if G is a tree, the above equality can be expressed as the Coulson integral:

$$E(G) = \frac{2}{\pi} \int_{0}^{+\infty} \frac{1}{x^2} \ln \left[1 + \sum_{j \geq 0} b_{2j}\, x^{2j} \right] \mathtt{dx} \tag{1}$$

where $b_{2j} = (-1)^j\, a_{2j}$. For more details on the graph energy see refs. [1, 17] and references therein.

Formula (1) makes it possible to compute the energy of trees without knowing the zeros of the characteristic polynomial, and hence is found many applications. For instance, let H_1 and H_2 be trees with n vertices, and suppose the coefficients b_j of these two trees satisfy

$$b_j(H_1) \leq b_j(H_2) \qquad \texttt{for all} \quad j = 1, \ldots, \left\lfloor \frac{n}{2} \right\rfloor .$$

Then from formula (1), it follows immediately that $E(H_1) \leq E(H_2)$ [18]. However, it is expressed as a complicated improper integral, and cannot show us a direct way to compute the energy of trees. Motivated by this, we introduce an auxiliary polynomial to calculate the energy of trees, and obtain a formula which depends on the coefficients of the characteristic polynomial, and thus enables one to calculate the energy of trees in a more direct way.

2 A formula for calculating the energy of trees

First, we list some preliminaries that will be used in what follows.

Lemma 2.1. [19, 20] If T is a tree with n vertices, then the characteristic polynomial $\phi(T, \lambda)$ can be expressed as

$$\phi(T, \lambda) = \sum_{j=0}^{\lfloor n/2 \rfloor} (-1)^j\, m(T, j)\, \lambda^{n-2j}$$

where $m(T,j)$ is the number of j-matchings of T. By convention, $m(T,0)=1$.

Lemma 2.2.(See [21].) The collection of all zeros of $\phi(T,\lambda)$ is symmetric with respect to the origin.

Define

$$f(x)=\sum_{j=0}^{n_0}(-1)^j\, m(T,j)\, x^{n_0-j}$$

where n_0 is the size of the maximal matching of T.

As an example for a tree $T^{(0)}$ (see Fig. 1), we have $f(x)=x^5-9x^4+26x^3-30x^2+13x-1$, which is directly calculated by a method similar to that in [22].

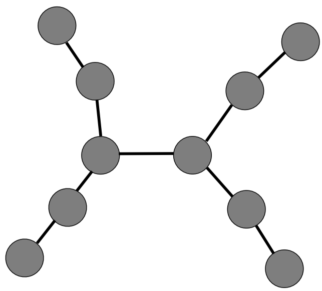

Figure 1: A tree $T^{(0)}$ with 10 vertices.

According to Lemmas 2.1 and 2.2, the following lemma is straightforward.

Lemma 2.3. (I) $\phi(T,\lambda)=\lambda^{m_0}f(\lambda^2)$, where m_0 is the nullity (= number of zero eigenvalues). (II) If x_k is a zero of $f(x)$, then both $\sqrt{x_k}$ and $-\sqrt{x_k}$ are zeros of $\phi(T,\lambda)$. (III) Each zero of $f(x)$ is a positive real number.

For $1\le j\le m$, denote a zero of $f(x)$ by x_j, whose multiplicity is m_j. As a consequence of Lemma 2.3, we obtain

$$E(T)=\sum_{j=1}^{m}2m_j\sqrt{x_j}\,. \tag{2}$$

In Eq. (2), we can evaluate the quantity m_j by the following method due to Guan [23].

Lemma 2.4. If m_j is the multiplicity of zero x_j of $f(x)$, then

$$m_j=\lim_{x\to x_j}\frac{(f'(x))^2}{(f'(x))^2-f(x)f''(x)}$$

where $f'(x)$, as usual, is the derivative of $f(x)$.

Proof. For completeness, we provide an independent proof. Since m_j is the multiplicity of zero x_j of $f(x)$, we can write $f(x)$ as $f(x) = f_1(x)f_2(x)$ with $f_1(x) = (x - x_j)^{m_j}$ and $f_2(x_j) \neq 0$. As a result, we have

$$\begin{aligned}\frac{f(x)f''(x)}{(f'(x))^2} &= \frac{f_1(x)f_2(x)\left[f_1''(x)f_2(x) + 2f_1'(x)f_2'(x) + f_1(x)f_2''(x)\right]}{\left(f_1'(x)f_2(x) + f_1(x)f_2'(x)\right)^2} \\ &= \frac{f_2(x)\left[m_j(m_j-1)f_2(x) + 2m_j(x-x_j)f_2'(x) + (x-x_j)^2 f_2''(x))\right]}{\left(m_j f_2(x) + (x-x_j)f_2'(x)\right)^2}.\end{aligned}$$

Taking a limit gives $\lim_{x\to x_j} \frac{f(x)f''(x)}{(f'(x))^2} = \frac{m_j-1}{m_j}$, and this leads to $\lim_{x\to x_j} \frac{(f'(x))^2}{(f'(x))^2 - f(x)f''(x)} = m_j$, as a desired value.

In order to obtain the quantity $\sqrt{x_j}$ in Eq. (2) for all $1 \le j \le m$, let $d(x)$ denote the greatest common factor between $f(x)$ and $f'(x)$, and set $g(x) = f(x)/d(x)$. Notice now that $g(x)$ is a polynomial of order m, whose zeros are $x_1, \ldots, x_m$ in which $x_j \neq x_k$ if and only if $j \neq k$. Therefore, $g(x)$ may read as $g(x) = x^m + c_1x^{m-1} + \cdots + c_m$.

Put $c_0 = 1$ for simplicity, and recursively define $c_{j,p}$ for all $0 \le j \le m$ and $p \ge 0$ as follows.

- If $p = 0$, $c_{j,p} = c_j$.
- If $p \ge 1$, $c_{j,p} = c_{j,p-1}^2 + 2\sum_{k\ge1}(-1)^k c_{j-k,p-1}c_{j+k,p-1}$, where "$j - k \ge 0$" and "$j + k \le m$" must hold.

Theorem 2.5. $\sqrt{x_j} = \lim_{p\to\infty} \sqrt[2q]{\frac{c_{j,p}}{c_{j-1,p}}}$ for all $1 \le j \le m$, where $q = 2^p$.

Proof. We follow Lobachevsky [24] to proceed the following equation

$$g(x) = x^m + c_1x^{m-1} + \cdots + c_m = 0 \tag{3}$$

and write it as

$$x^m + c_1x^{m-1} + \cdots + c_m = (x - x_1)(x - x_2)\cdots(x - x_m) = 0\,. \tag{4}$$

Replacing x with $-x$ gives

$$x^m - c_1x^{m-1} + c_2x^{m-2} + \cdots + (-1)^m c_m = (x + x_1)(x + x_2)\cdots(x + x_m) = 0\,. \tag{5}$$

Combining Eq. (4) with Eq. (5) gets $(x^2 - x_1^2)(x^2 - x_2^2)\cdots(x^2 - x_m^2) = 0$, and further becomes

$$(z - x_1^2)(z - x_2^2)\cdots(z - x_m^2) = 0 \tag{6}$$

where $z = x^2$.

On the other hand, multiplying the left-hand sides of the two Eqs. (4) and (5), we obtain

$$\begin{array}{llllll}
\multicolumn{6}{c}{\left(c_0x^m + c_1x^{m-1} + \cdots + c_m\right) \times \left(c_0x^m - c_1x^{m-1} + \cdots + (-1)^m c_m\right)} \\
= c_0^2x^{2m} & + c_0c_1 \quad x^{2m-1} & - c_1^2 \quad x^{2m-2} & - c_0c_3 \quad x^{2m-3} & + c_2^2 \quad x^{2m-4} & - \cdots = 0. \\
 & -c_0c_1 & +c_0c_2 & +c_1c_2 & -c_1c_3 & \\
 & & +c_0c_2 & -c_1c_2 & -c_1c_3 & \\
 & & & +c_0c_3 & +c_0c_4 & \\
 & & & & +c_0c_4 &
\end{array}$$

Then substituting z for x^2 gives

$$c_0^2z^m + (-c_1^2 + 2c_0c_2)z^{m-1} + (c_2^2 - 2c_1c_3 + 2c_0c_4)z^{m-2} + \cdots = 0\,.$$

Together with (6), we have

$$\begin{aligned}
& c_0^2z^m + (-c_1^2 + 2c_0c_2)z^{m-1} + (c_2^2 - 2c_1c_3 + 2c_0c_4)z^{m-2} + \cdots \\
= \;& c_0^2(z - x_1^2)(z - x_2^2)\cdots(z - x_m^2) \\
= \;& 0\,.
\end{aligned}$$

Herein changing z into $-z$ yields

$$\begin{aligned}
& c_0^2z^m + (c_1^2 - 2c_0c_2)z^{m-1} + (c_2^2 - 2c_1c_3 + 2c_0c_4)z^{m-2} + \cdots \\
= \;& c_0^2(z + x_1^2)(z + x_2^2)\cdots(z + x_m^2) \\
= \;& 0\,.
\end{aligned} \tag{7}$$

In Eq.(7), the coefficient of z^k is obtained from the coefficients in Eq. (3) by taking the square of the coefficient of x^k, minus twice the product of two coefficients of x^{k-1} and x^{k+1}, plus twice the product of two coefficients of x^{k-2} and x^{k+2}, and so on, until the coefficient of the first item or last item appears.

If we proceed Eq. (7) analogous to Eq. (3), we shall obtain a new equation of order m, whose roots are $-x_1^4,\ -x_2^4,\ \cdots,\ -x_m^4$. We say that the original Eq. (3) is proceeded twice. Proceeding the original Eq. (3) p times, we arrive at a new equation

$$c_{0,p}x^m + c_{1,p}x^{m-1} + \cdots + c_{m,p} = 0$$

whose roots are $-x_1^q,\ -x_2^q,\ \ldots,\ -x_m^q$, where $c_{j,p}$ for all $0 \le j \le m$ and $p \ge 0$ is defined as above.

Bearing in mind that $c_{0,p}x^m + c_{1,p}x^{m-1} + \cdots + c_{m,p} = c_{0,p}(x+x_1^q)(x+x_2^q)\cdots(x+x_m^q) = 0$ and $c_{0,p} = 1$, we obtain

$$\begin{cases} x_1^q + \cdots + x_m^q = c_{1,p} \\ (x_1x_2)^q + (x_1x_3)^q + \cdots = c_{2,p} \\ (x_1x_2x_3)^q + (x_1x_2x_4)^q + \cdots = c_{3,p} \\ \cdots\cdots \\ (x_1x_2\cdots x_m)^q = c_{m,p} \end{cases}.$$

Assume that $x_1 > x_2 > \cdots > x_m > 0$, and write the above equalities as

$$\left.\begin{array}{c} (\sqrt{x_1})^{2q}\left[1 + (\sqrt{\frac{x_2}{x_1}})^{2q} + \cdots + (\sqrt{\frac{x_m}{x_1}})^{2q}\right] = c_{1,p} \\ (\sqrt{x_1x_2})^{2q}\left[1 + (\sqrt{\frac{x_3}{x_2}})^{2q} + \cdots\right] = c_{2,p} \\ (\sqrt{x_1x_2x_3})^{2q}\left[1 + (\sqrt{\frac{x_4}{x_3}})^{2q} + \cdots\right] = c_{3,p} \\ \cdots\cdots \\ (\sqrt{x_1x_2\cdots x_m})^{2q} = c_{m,p} \end{array}\right\}.$$

Since the absolute values of the fractions $\frac{x_2}{x_1}, \frac{x_3}{x_1}, \cdots, \frac{x_m}{x_{m-1}}$ are less than 1, there is always the index q such that the quantities $\left(\sqrt{\frac{x_2}{x_1}}\right)^{2q}, \left(\sqrt{\frac{x_3}{x_1}}\right)^{2q}, \ldots, \left(\sqrt{\frac{x_m}{x_{m-1}}}\right)^{2q}$ are omitted within the error range. Thus we obtain

$$\begin{cases} (\sqrt{x_1})^{2q} = c_{1,p} \\ (\sqrt{x_1x_2})^{2q} = c_{2,p} \\ (\sqrt{x_1x_2x_3})^{2q} = c_{3,p} \\ \cdots\cdots \\ (\sqrt{x_1x_2\cdots x_m})^{2q} = c_{m,p} \end{cases} \tag{8}$$

followed by

$$\begin{cases} (\sqrt{x_1})^{2q} = c_{1,p} \\ (\sqrt{x_2})^{2q} = \frac{c_{2,p}}{c_{1,p}} \\ \cdots\cdots \\ (\sqrt{x_m})^{2q} = \frac{c_{m,p}}{c_{m-1,p}} \end{cases}$$

further implying

$$\sqrt{x_j} = \lim_{p\to\infty} \sqrt[2q]{\frac{c_{j,p}}{c_{j-1,p}}} \tag{9}$$

for all $1 \leq j \leq m$.

From Lemma 2.4 and Theorem 2.5, we have obtained a novel method for calculating a value for $E(T)$.

Theorem 2.6. Suppose that $f(x) = \sum_{j=0}^{n_0}(-1)^j\, m(T,j)\, x^{n_0-j}$, $d(x)$ =the greatest common factor between $f(x)$ and its derivative $f'(x)$, and $g(x) = f(x)/d(x) = c_0x^m + c_1x^{m-1} + \cdots + c_m$. Then,

$$E(T) = \sum_{j=1}^{m} 2m_j\sqrt{x_j} = \lim_{p\to\infty}\sum_{j=1}^{m}\frac{2(f'(x_{j,p}))^2}{(f'(x_{j,p}))^2 - f(x_{j,p})f''(x_{j,p})}\sqrt{x_{j,p}} \tag{10}$$

where $m_j = \lim_{p\to\infty}\frac{(f'(x_{j,p}))^2}{(f'(x_{j,p}))^2-f(x_{j,p})f''(x_{j,p})}$, $\sqrt{x_j} = \lim_{p\to\infty}\sqrt{x_{j,p}}$, and $x_{j,p} = \sqrt[q]{\frac{c_{j,p}}{c_{j-1,p}}}$ in which q is equal to 2^p, and $c_{j,p}$ for all $0 \le j \le m$ and $p \ge 0$ is recursively defined as follows: if $p = 0$, $c_{j,p} = c_j$; if $p \ge 1$, $c_{j,p} = c_{j,p-1}^2 + 2\sum_{k\ge1}(-1)^k c_{j-k,p-1}c_{j+k,p-1}$, and the summation $\sum_{k\ge1}$ is over "$j-k \ge 0$" and "$j+k \le m$".

Remark 2.7. In practice, there should be a more detailed explanation how to use Eq. (10) to get the approximate value for $E(T)$. First, in view of Eq. (10), we have

$$E(T) \approx E(T_p) := \sum_{j=1}^{m}\frac{2(f'(x_{j,p}))^2}{(f'(x_{j,p}))^2 - f(x_{j,p})f''(x_{j,p})}\sqrt{x_{j,p}} \tag{11}$$

and use it to obtain an approximation of $E(T)$ with any given precision just by choosing the appropriate parameter p. For convenience we take $c_0 = 1$, giving rise to $c_{0,p} = 1$ for all $p \ge 1$. Then from Eq. (8) when the parameter p is replaced by $p+1$, it follows that $\left((\sqrt{x_1\cdots x_j})^{2q}\right)^2 = \frac{c_{j,p+1}}{c_{0,p+1}} = c_{j,p+1}$ for all $1 \le j \le m$. This and the relations $(\sqrt{x_1\cdots x_j})^{2q} = \frac{c_{j,p}}{c_{0,p}} = c_{j,p}$ jointly produce $(c_{j,p})^2 = c_{j,p+1}$, i.e.,

$$2\lg(c_{j,p}) = \lg(c_{j,p+1})$$

for all $1 \le j \le m$. Thus, the quantities $c_{j,p}$ are desired values as suggested in [24], once the above equations for all $1 \le j \le m$ are satisfied. Next, the multiplicity m_j of zero x_j of $f(x)$ is exactly equal to the integer nearest to the real number $\frac{(f'(x_{j,p}))^2}{(f'(x_{j,p}))^2-f(x_{j,p})f''(x_{j,p})}$, which follows from Lemma 2.4.

It is worth mentioning that $\sqrt{x_j}$ for each $1 \le j \le m$ is actually the j-th eigenvalue [25,26] of T, and Eq. (9) is a new method for calculating the eigenvalues of T. Compared to the existing methods [27–29], our method is of interest in its own right.

3 An example

We choose again the tree $T^{(0)}$ (see Fig. 1) to demonstrate the method in Eq. (11). By a direct calculation, we obtain the related functions as follows: $f(x) = (x-1)^2(x^3 - 7x^2 +$

$11x-1) = x^5 - 9x^4 + 26x^3 - 30x^2 + 13x - 1$, $f'(x) = (x-1)(5x^3 - 31x^2 + 47x - 13)$, $f''(x) = 20x^3 - 108x^2 + 156x - 60$, $d(x) = x - 1$, and $g(x) = f(x)/d(x) = (x-1)(x^3 - 7x^2 + 11x - 1) = x^4 - 8x^3 + 18x^2 - 12x + 1$. Table 1 displays the approximate values $E(T_p^{(0)})$ for $p = 1$ through 6.

Table 1: Calculating the approximate values $E(T_p^{(0)})$ for $p = 1$ through 6 with initial conditions $c_{0,0} = 1$, $c_{1,0} = -8$, $c_{2,0} = 18$, $c_{3,0} = -12$ and $c_{4,0} = 1$.

	$\sqrt[2q]{\frac{c_{1,p}}{c_{0,p}}}$	$\sqrt[2q]{\frac{c_{2,p}}{c_{1,p}}}$	$\sqrt[2q]{\frac{c_{3,p}}{c_{2,p}}}$	$\sqrt[2q]{\frac{c_{4,p}}{c_{3,p}}}$	$E(T_p^{(0)})$
$p=1$	2.3003266338	1.4790630640	0.9475011359	0.31020161970	12.0741849068
$p=2$	2.1831381187	1.4804977697	0.9945006811	0.31110425063	11.9384816402
$p=3$	2.1703876992	1.4811614118	0.9998834217	0.31110781732	11.9250806999
$p=4$	2.1700868205	1.4811942368	0.9999998915	0.31110781747	11.9247775328
$p=5$	2.1700864866	1.4811943041	1.0000000000	0.31110781747	11.9247772164
$p=6$	2.1700864866	1.4811943041	1.0000000000	0.31110781747	11.9247772164

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