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Spectral moments of trees with given degree sequence

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ABSTRACT

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of a graph G. For any $k \geqslant 0$, the k-th spectral moment of G is defined by $\mathrm{M}_k(G) = \lambda_1^k + \dots + \lambda_n^k$. We use the fact that $\mathrm{M}_k(G)$ is also the number of closed walks of length k in G to show that among trees T whose degree sequence is D or majorized by D, $\mathrm{M}_k(T)$ is maximized by the greedy tree with degree sequence D (constructed by assigning the highest degree in D to the root, the second-, third-, …highest degrees to the neighbors of the root, and so on) for any $k \geqslant 0$. Several corollaries follow, in particular a conjecture of Ilić and Stevanović on trees with given maximum degree, which in turn implies a conjecture of Gutman, Furtula, Marković and Glišić on the Estrada index of such trees, which is defined as $\mathrm{EE}(G) = e^{\lambda_1} + \dots + e^{\lambda_n}$.

1. Introduction

Let G be a graph with adjacency matrix A, and let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A. The k-th spectral moment of G is defined as

$$\mathrm{M}_k(G) = \sum_{k=0}^{n} \lambda_i^k. \tag{1}$$

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A *walk* of length k in a graph G is any sequence $w_1 w_2 \ldots w_{k+1}$ of vertices of G such that $w_i w_{i+1}$ is an edge in G for $i = 1, \ldots, k$. Since $\mathrm{tr}(A^k) = \mathrm{M}_k(G)$, where $\mathrm{tr}(A^k)$ is the trace of the k-th power of A, $\mathrm{M}_k(G)$ is (see [5]) exactly the number of closed walks (walks that start and end at the same vertex) of length k in G. The spectral moments of G are also closely related to the so-called *Estrada index* [6], which is defined as

$$\mathrm{EE}(G) = \sum_{i=1}^{n} e^{\lambda_i}. \tag{2}$$

It follows from (1), (2) and the power series expansion of the exponential function that

$$\mathrm{EE}(G) = \sum_{i=1}^{n} \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{k=0}^{\infty} \frac{\mathrm{M}_k(G)}{k!}. \tag{3}$$

Ernesto Estrada [11] introduced the parameter EE in 2000 and showed how it can be used to study aspects of molecular structures such as the degree of folding of proteins, see also [12,13]. Applications of EE expanded quickly to the study of complex networks [14] and quantum chemistry [15]. See [17] for a recent survey on the Estrada index.

Let us also define a generalization of the graph invariant EE: for any function $f : \mathbb{R} \to \mathbb{R}$, we set

$$\mathrm{E}_f(G) = \sum_{i=1}^{n} f(\lambda_i). \tag{4}$$

Obviously, we obtain the k-th spectral moment for $f(x) = x^k$, the Estrada index for $f(x) = e^x$ and the graph energy (see [21] and the references therein) for $f(x) = |x|$. More examples will be discussed at a later stage. If we assume that f has a power series expansion around 0 that converges everywhere, i.e.,

$$f(x) = \sum_{k=0}^{\infty} a_k x^k, \tag{5}$$

then E_f satisfies the relation

$$\mathrm{E}_f(G) = \sum_{i=1}^{n} \sum_{k=0}^{\infty} a_k \lambda_i^k = \sum_{k=0}^{\infty} a_k \mathrm{M}_k(G). \tag{6}$$

Let $\mathbb{T}_D$ denote the set of trees with degree sequence D. The class of trees with fixed degree sequence is very popular in extremal graph theory. For example, it has been studied with regards to the Wiener index [24,25] and other distance-based invariants [22], spectral radius and Laplacian spectral radius [3,4,27], the energy and the number of independent subsets [1], and the number of subtrees [28,29].

The greedy tree $G(D)$ is the tree obtained from a "greedy algorithm" that we will describe in detail in the following section. Roughly speaking, it is obtained by assigning the highest degree in D to the root, the largest degrees that are left to its neighbors, and so on.

For any degree sequence D, we prove that $G(D)$ has maximum k-th spectral moment for any $k \geqslant 0$, and for sufficiently large k, it is unique with this property. Consequently, the greedy tree also maximizes E_f for any f as in (5) among all elements of $\mathbb{T}_D$, provided that the coefficients a_k are nonnegative for even k (the odd spectral moments are 0 for all bipartite graphs, thus in particular for trees). Details of the proof are provided in Section 3. Furthermore, in Section 4 we show that if two degree sequences $D = (d_1, \ldots, d_n)$ and $B = (b_1, \ldots, b_n)$ satisfy

$$\sum_{i=1}^{l} b_i \leqslant \sum_{i=1}^{l} d_i \tag{7}$$