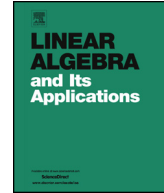




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Spectral moments of trees with given degree sequence



Eric Ould Dadah Andriantiana¹, Stephan Wagner^{*,2}

Department of Mathematical Sciences, Stellenbosch University, Private Bag X1, Matieland 7602, South Africa

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ABSTRACT

Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of a graph G . For any $k \geq 0$, the k -th spectral moment of G is defined by $M_k(G) = \lambda_1^k + \dots + \lambda_n^k$. We use the fact that $M_k(G)$ 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 , $M_k(T)$ 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 $k \geq 0$. 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 $EE(G) = e^{\lambda_1} + \dots + e^{\lambda_n}$.

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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

$$M_k(G) = \sum_{i=1}^n \lambda_i^k. \quad (1)$$

* Corresponding author.

E-mail addresses: ericoda@sun.ac.za (E.O.D. Andriantiana), swagner@sun.ac.za (S. Wagner).

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A walk of length k in a graph G is any sequence $w_1 w_2 \dots w_{k+1}$ of vertices of G such that $w_i w_{i+1}$ is an edge in G for $i = 1, \dots, k$. Since $\text{tr}(A^k) = M_k(G)$, where $\text{tr}(A^k)$ is the trace of the k -th power of A , $M_k(G)$ 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

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

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

$$EE(G) = \sum_{i=1}^n \sum_{k=0}^{\infty} \frac{\lambda_i^k}{k!} = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}. \quad (3)$$

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 $f: \mathbb{R} \rightarrow \mathbb{R}$, we set

$$E_f(G) = \sum_{i=1}^n f(\lambda_i). \quad (4)$$

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.,

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

then E_f satisfies the relation

$$E_f(G) = \sum_{i=1}^n \sum_{k=0}^{\infty} a_k \lambda_i^k = \sum_{k=0}^{\infty} a_k M_k(G). \quad (6)$$

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 $k \geq 0$, 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 $D = (d_1, \dots, d_n)$ and $B = (b_1, \dots, b_n)$ satisfy

$$\sum_{i=1}^l b_i \leq \sum_{i=1}^l d_i \quad (7)$$

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