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On the A_α-characteristic polynomial of a graph
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Let G be a simple graph with vertex set $V(G)$. The *adjacency matrix* of G is the $(0,1)$-matrix $A(G) = (a_{uv})_{u,v\in V(G)}$, where $a_{uv} = 1$ if u is adjacent to v, and 0 otherwise. Let $d(v)$ be the degree of vertex v in G, and let $D(G) = \mathrm{diag}(d(v) : v \in V(G))$. The A_α-*matrix* of G, introduced by Nikiforov [1], is defined as $A_\alpha(G) = \alpha D(G)+(1-\alpha)A(G)$, where $\alpha \in [0,1]$ is a real number. In particular, $A_0(G) = A(G)$, and $2A_{\frac{1}{2}}(G) = Q(G)$ is just the *signless Laplacian matrix* of G. The A_α-*characteristic polynomial* of G is defined as $\phi(A_\alpha(G); x) = \det(xI - A_\alpha(G))$, where I denotes the identity matrix. Two graphs G and H are called A_α-*cospectral* if $\phi(A_\alpha(G); x) = \phi(A_\alpha(H); x)$ (here α is considered as an indeterminate). A graph G is called A_α-*DS* if any other graph A_α-cospectral with G must be isomorphic to it.

This paper contains mainly two parts. In the first part, the authors formulate the first four coefficients of the A_α-characteristic polynomial of G.

Theorem 1. *Let G be a graph with n vertices, m edges and t_G triangles, and let $\deg(G) = (d_1, d_2, \ldots, d_n)$ be its degree sequence. Suppose that $\phi(A_\alpha(G); x) = \sum_{j=0}^{n} c_{\alpha j}(G)x^{n-j}$. Then*

$$c_{\alpha 0}(G) =1,\ c_{\alpha 1}(G) = -2\alpha m,\ c_{\alpha 2}(G) = 2\alpha^2m^2 - (1-\alpha)^2m - \frac{1}{2}\alpha^2\sum_{r=1}^{n} d_r^2,$$

$$c_{\alpha 3}(G) = -\frac{1}{3}\left(6(1-\alpha)^3 t_G - 6\alpha(1-\alpha)^2 m^2 + 3\alpha(1-\alpha)^2 \sum_{r=1}^{n} d_r^2 \right.$$
$$\left. +\alpha^3\left(4m^3 - 3m\sum_{r=1}^{n} d_r^2 + \sum_{r=1}^{n} d_r^3\right)\right).$$

Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ denote the eigenvalues of $A_\alpha(G)$. As a corollary of Theorem 1, the authors obtain that

Corollary 2. *Let G and $\phi(A_\alpha(G); x)$ be as in Theorem 1. Then*

$$c_{\alpha 0}(G) = 1,\ c_{\alpha 1}(G) = -\sum_{i=1}^{n} \lambda_i = -\mathrm{tr}(A_\alpha(G)),$$
$$c_{\alpha 2}(G) = 2\alpha^2 m^2 - \frac{1}{2}\sum_{i=1}^{n} \lambda_i^2 = 2\alpha^2 m^2 - \frac{1}{2}\mathrm{tr}(A_\alpha^2(G)),$$
$$c_{\alpha 3}(G) = -\frac{1}{3}\left(\sum_{i=1}^{n} \lambda_i^3 - 3\alpha m \sum_{i=1}^{n} \lambda_i^2 + 4\alpha^3 m^3\right)$$
$$= -\frac{1}{3}\left(\mathrm{tr}(A_\alpha^3(G)) - 3\alpha m\,\mathrm{tr}(A_\alpha^2(G)) + 4\alpha^3 m^3\right).$$

In the second part, the authors focus on the following problem proposed by van Dam and Haemers [2]:

Problem 3. *Which linear combination of $D(G)$, $A(G)$, and J (all ones matrix) gives the most DS graphs?*

Concretely, the authors enumerate the A_α-characteristic polynomials for all graphs on at most 10 vertices. The computational data shows that there are no non-isomorphic A_α-cospectral graphs for $n \leq 8$, and exactly 2 and 10146 graphs with A_α-cospectral mate for $n = 9$ and $n = 10$, respectively. These results suggest that A_α-characteristic polynomials are much more efficient than A- and Q-characteristic polynomials to distinguish graphs.

References

[1] V. Nikiforov, Merging the A- and Q-spectral theories, Appl. Anal. Discrete Math. 11 (2017) 81–107.

[2] E.R. van Dam, W.H. Haemers, Which graphs are determined by their spectrum?, Linear Algebra Appl. 373 (2003) 241–272.