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# Constructions of Graphs and Trees with Partially Prescribed Spectrum

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#### Abstract

It is shown how a connected graph and a tree with partially prescribed spectrum can be constructed. These constructions are based on a recent result of Salez that every totally real algebraic integer is an eigenvalue of a tree. Our result implies that for any (not necessarily connected) graph, there is a tree such that the characteristic polynomial of the graph divides the characteristic polynomial of the tree.

#### 1 Introduction

Graph eigenvalues have been studied intensively [1–3], and they are very special real numbers. Indeed, they are totally real algebraic integers, i.e., roots of totally real algebraic polynomials. Recall that a *totally real algebraic polynomial* is a monic integral polynomial with only real roots. It is natural for one to wonder whether the converse is true. Forty years ago, Hoffman [6] conjectured that this is true, which eventually was confirmed by Estes [4] in 1992.

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**Theorem 1.** [4] Every totally real algebraic integer is an eigenvalue of a (connected) graph.

Recently, Salez [7] strengthened the result with a simpler proof.

**Theorem 2.** [7] Every totally real algebraic integer is an eigenvalue of a tree.

The next natural question is which collection of totally real algebraic integers forms the spectrum of a graph. Of course, there are many necessary conditions on such a collection. Below, we list just a few.

**Lemma 3.** If  $S = \{\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n\}$  is the spectrum of a graph of order n, then

- 1. S contains all the conjugates of each  $\lambda_i$ ,
- 2.  $\lambda_1 + \cdots + \lambda_n = 0$ ,
- 3.  $\lambda_1^2 + \dots + \lambda_n^2 \le n(n-1),$
- 4.  $\lambda_1 \le n 1$ ,
- 5.  $|\lambda_n| \leq \lambda_1$ .

Unfortunately, these conditions are far from being sufficient, as the next example shows.

**Example 4.** The set  $\{2, 1, -1, -2\}$  satisfies all the conditions listed in Lemma 3, but it is not the spectrum of any graph of order 4.

*Proof.* Suppose that there is a graph G of order 4 with the spectrum

$$Spec(G) = \{2, 1, -1, -2\}.$$

Then G is bipartite because Spec(G) is symmetric about 0. Hence the number of edges of G is at most 4 because G is a bipartite graph of order 4. On the other hand, the number of edges of G, computed by means of its eigenvalues, would be  $\frac{1}{2}[2^2+1^2+(-1)^2+(-2)^2]=5$ , a contradiction!

The problem of finding necessary and sufficient conditions for a set of totally real algebraic integers to be the spectrum of a graph seems intractable! Instead, we tackle its following modification: **Problem 5.** Construct a connected graph such that its spectrum contains a given set of totally real algebraic integers.

In Section 2, we accomplish such a construction via Knonecker product of matrices. In Section 3, we strengthen the result by constructing a tree via an appropriate graph operation. Then we discuss the unimodalization of totally real algebraic polynomials.

## 2 Construction of connected graphs

Recall some facts about the Kronecker product of matrices:

Fact 1:  $Spec(A \otimes B) = \{\alpha\beta : \alpha \in Spec(A), \beta \in Spec(B)\}.$ 

Fact 2:  $Spec(A \otimes I + I \otimes B) = \{\alpha + \beta : \alpha \in Spec(A), \beta \in Spec(B)\}.$ 

Fact 3: If A and B are adjacency matrices, then  $A \otimes B$  is also an adjacency matrix.

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In view of Facts 3 and 4, we introduce two graph products as follows:

**Definition 6.** Given two graphs G and H, define a new graph G + H such that its adjacency matrix is given by  $A(G + H) = A(G) \otimes I + I \otimes A(H)$ .

**Definition 7.** Given two graphs G and H, define a new graph  $G \times H$  such that its adjacency matrix is given by  $A(G \times H) = A(G) \otimes A(H)$ .

Using Facts 1 and 2, we have

$$Spec(G + H) = Spec(G) + Spec(H)$$

and

$$Spec(G \times H) = Spec(G) \cdot Spec(H)$$
.

Moreover, if G and H are connected, then G + H is also connected. It is well known that  $G \times H$  is connected if and only if both G and H are connected, and one of G and H contains a cycle of odd length, i.e., one of them is non-bipartite.

**Lemma 8.** Given a connected graph G such that  $\alpha \in Spec(G)$ . Then there is a connected graph H such that  $0, \alpha \in Spec(H)$ .

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Proof. Consider the graph  $F = P_5 + C_3$ , where the path  $P_5$  of order 5 has  $Spec(P_5) = \{\sqrt{3}, 1, 0, -1, -\sqrt{3}\}$ , and the cycle  $C_3$  of order 3 has  $Spec(C_3) = \{2, -1, -1\}$ . Then F has eigenvalues 0 = 1 + (-1) and 1 = (-1) + 2. Moreover, F is connected and non-bipartite since it contains an odd cycle  $C_3$ . Now take  $H = F \times G$ . Then H is connected and  $0, \alpha \in Spec(H)$ .

**Remark 9.** In the proof of Lemma 8, it is possible to use another F of smaller order and size with the required properties: connected, non-bipartite, and  $0, 1 \in Spec(F)$ . For example, take F to be the graph obtained by attaching two pendent vertices and a 2-vertex path to the same vertex of a triangle.

**Theorem 10.** Let  $\alpha_1, \ldots, \alpha_p$  be totally real algebraic integers. Then there is a connected graph H such that  $\{\alpha_1, \ldots, \alpha_p\} \subseteq Spec(H)$ .

*Proof.* We prove, by induction on p, a stronger statement: There is a connected graph H such that  $\{0, \alpha_1, \ldots, \alpha_p\} \subseteq Spec(H)$ .

Consider p = 1. By Theorem 1, there is a graph G such that  $\alpha_1 \in Spec(G)$ . Without loss of generality, we can assume that G is connected. Now, by Lemma 8, there is a connected graph H such that  $0, \alpha_1 \in Spec(H)$ .

Consider p > 1. By the induction assumption, there is a connected graph K such that  $\{0, \alpha_1, \ldots, \alpha_{p-1}\} \subseteq Spec(K)$ . Applying the case p = 1, we have a connected graph G such that  $0, \alpha_p \in Spec(G)$ . Take H = K + G. Then H is connected because both K and G are connected. Moreover,

$$0, \alpha_1, \dots, \alpha_{p-1}, \alpha_p \in \{0, \alpha_1, \dots, \alpha_{p-1}\} + \{0, \alpha_p\} \subseteq Spec(K) + Spec(G) = Spec(H).$$

### **3** Construction of trees

We start this section with a lemma on the spectrum of a special type of block matrices.

Lemma 11. Let A and B be square matrices. Then

$$Spec\left(\left[\begin{array}{ccc} A & F & F \\ E & B & 0 \\ E & 0 & B \end{array}\right]\right) = Spec(B) \bigcup Spec\left(\left[\begin{array}{ccc} A & 2F \\ E & B \end{array}\right]\right).$$

Proof. Note that

$$\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & I & I \end{bmatrix} = \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & -I & I \end{bmatrix}^{-1}$$

Then the following matrix identity is in fact a similarity transformation:

$$\begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & -I & I \end{bmatrix} \begin{bmatrix} A & F & F \\ E & B & 0 \\ E & 0 & B \end{bmatrix} \begin{bmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & I & I \end{bmatrix} = \begin{bmatrix} A & 2F & F \\ E & B & 0 \\ 0 & 0 & B \end{bmatrix}.$$
  
Therefore, 
$$\begin{bmatrix} A & F & F \\ E & B & 0 \\ E & 0 & B \end{bmatrix}$$
 and 
$$\begin{bmatrix} A & 2F & F \\ E & B & 0 \\ 0 & 0 & B \end{bmatrix}$$
 have the same spectrum, and so the conclusion follows.

Given disjoint graphs G,  $H_i$ , and  $H'_i$  such that  $H_i$  and  $H'_i$  are isomorphic for i = 1, 2, ..., p. Let  $x_i$ , i = 1, 2, ..., p, be vertices of G (not necessarily different). Let  $v_i$  be a vertex of  $H_i$ , and  $v'_i$  a vertex of  $H'_i$ . Construct a graph  $G \circ [H_1, \cdots, H_p]$  by connecting  $x_i$  to both  $v_i$  and  $v'_i$  with new edges, for i = 1, 2, ..., p.

Lemma 12.  $Spec(H_1 \cup \cdots \cup H_p) \subseteq Spec(G \circ [H_1, \cdots, H_p]).$ 

*Proof.* Let  $H = H_1 \cup \cdots \cup H_p$  and  $H' = H'_1 \cup \cdots \cup H'_p$ . Since  $H_i$  and  $H'_i$  are isomorphic, H and H' are also isomorphic. Hence, by a suitable labeling, we have A(H) = A(H') and

$$A(G \circ [H_1, \cdots, H_p]) = \begin{bmatrix} A(G) & E^T & E^T \\ E & A(H) & 0 \\ E & 0 & A(H) \end{bmatrix}.$$

Consequently, by Lemma 11,

$$\begin{aligned} Spec(H_1 \cup \dots \cup H_p) &= Spec(H) \\ &= Spec(A(H)) \\ &\subseteq Spec(A(G \circ [H_1, \dots, H_p])) \\ &= Spec(G \circ [H_1, \dots, H_p]) \,. \end{aligned}$$

**Theorem 13.** Let  $\alpha_1, \ldots, \alpha_p$  be totally real algebraic integers. Then there is a tree T such that  $\{\alpha_1, \ldots, \alpha_p\} \subseteq Spec(T)$ .

*Proof.* For each totally real algebraic integer  $\alpha_i$ , by Theorem 2, there is a tree  $T_i$  whose spectrum contains  $\alpha_i$ . Take G to be any tree (say, just a singleton). By Lemma 12,  $Spec(T_1 \cup \cdots \cup T_p) \subseteq Spec(G \circ [T_1, \cdots, T_p])$  and so

$$\{\alpha_1,\ldots,\alpha_p\}\subseteq Spec(G\circ[T_1,\cdots,T_p]).$$

Moreover,  $T = G \circ [T_1, \cdots, T_p]$  is a tree because G and  $T_i$  are all trees.

**Example 14.** Note that  $Spec(K_2) = \{1, -1\}$ , and  $Spec(K_{1,4}) = \{2, 0, 0, 0, -2\}$ . Hence, by the construction in the proof of Theorem 13,  $K_1 \circ [K_2, K_{1,4}]$  is a tree whose spectrum contains  $\{2, 1, -1, -2\}$ .

A k-matching of a graph G is a set of k edges such that any two distinct edges in the set do not have a common end-point. The matching polynomial  $P_M(G, x)$  of G is defined as

$$P_M(G, x) = \sum_{k \ge 0} (-1)^k m(G, k) x^{n-2k}$$

where m(G, k) denotes the number of k-matchings in G with the convention m(G, 0) = 1. For matching polynomials, we know [2,5] that for any (not necessarily connected) graph G, the roots of  $P_M(G, x)$  are totally real algebraic integers, and moreover, there is a tree T such that  $P_M(G, x)$  is a divisor of  $P_M(T, x)$ . The next result says that a similar statement holds for the characteristic polynomials of graphs.

**Corollary 15.** For any (not necessarily connected) graph G, there is a tree T such that the characteristic polynomial P(G, x) of G divides the characteristic polynomial P(T, x)of T, i.e., P(G, x) is a divisor of P(T, x).

*Proof.* Since all the roots of P(G, x) are totally real algebraic integers, by Theorem 13 there is a tree T whose spectrum contains all the roots of P(G, x), and hence the conclusion follows.

A real polynomial is said to be *unimodal* if the sequence of its coefficients is unimodal, i.e., first increases and then decreases with only one peak.

**Corollary 16.** For any totally real algebraic polynomial f(x), there is another totally real algebraic polynomial g(x) such that f(x)g(x) is unimodal.

*Proof.* From Theorem 13, we know that f(x) is a divisor of the characteristic polynomial of a tree. Thus, we can choose a totally real algebraic polynomial g(x) so that f(x)g(x) is the characteristic polynomial of a tree. It is well known that the sequence of coefficients of the characteristic polynomial of any tree is unimodal [8]. The conclusion follows immediately.

This result means that any totally real algebraic polynomial can be unimodalized. For example, the characteristic polynomial of an arbitrary graph is usually not unimodal, but it can be unimodalized by another totally real algebraic polynomial. It could be an interesting question to ask how to unimodalize a totally real algebraic polynomial by using a totally real algebraic polynomial with the lowest possible degree.

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# References

- [1] A. E. Brouwer, W. H. Haemers, Spectra of Graphs, Springer, New York, 2012.
- [2] D. M. Cvetković, M. Doob, I. Gutman, A. Torgašev, Recent Results in the Theory of Graph Spectra, North-Holland, Amsterdam, 1988.
- [3] D. M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Applications, Barth, Heidelberg, 1995.
- [4] D. R. Estes, Eigenvalues of symmetric integer matrices, J. Number Theory 42 (1992) 292–296.
- [5] I. Gutman, A survey on the matching polynomial, in: Y. Shi, M. Dehmer, X. Li, I. Gutman (Eds.), *Graph Polynomials*, CRC Press, Boca Raton, 2016, pp. 77–99.
- [6] A. J. Hoffman, Eigenvalues of graphs, in: D. R. Fulkerson (Ed.), Studies in Graph Theory, Part II, Math. Assoc. Amer., Washington, 1975, pp. 225–245.
- [7] J. Salez, Every totally real algebraic integer is a tree eigenvalue, J. Comb. Theory B 111 (2015) 249–256.
- [8] A. J. Schwenk, On unimodal sequences of graphical invariants, J. Comb. Theory B 30 (1981) 247–250.