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Tree decomposition by eigenvectors

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Abstract

In this work a composition–decomposition technique is presented that correlates tree eigenvectors with certain eigenvectors of an associated so-called skeleton forest. In particular, the matching properties of a skeleton determine the multiplicity of the corresponding tree eigenvalue. As an application a characterization of trees that admit eigenspace bases with entries only from the set $\{0, 1, -1\}$ is presented. Moreover, a result due to Nylen concerned with partitioning eigenvectors of tree pattern matrices is generalized.

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Keywords: Tree; Eigenvector; Null space; Basis; Matching

1. Introduction

Eigenspaces of graphs have been researched to some degree since many years. This is especially the case for the null space, which has been studied for a number of graph classes. Compared to the amount of research spent on the spectrum of graphs, only little attention has been given to what the eigenvectors of graphs really look like. There exist explicit results on paths, cycles, circulant graphs, graph products and some other graph classes (see e.g. [1,2]).

This work investigates eigenvectors of trees. The eigenvectors of a graph, i.e. eigenvectors of the adjacency matrix, can be considered as real valued functions on its vertex set. One may partition the vertices of a tree by grouping those vertices on which there exist non-zero values for

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some vector from a fixed eigenspace and those on which every vector from that space vanishes. Then the components arising from vertices of the first kind can be contracted into single vertices (these components are loosely related to the so-called nut graphs studied in [3,4]). Together with any adjacent vertices they induce a so-called skeleton forest, a concept initially hinted at in [5]. We show that the null space of this skeleton provides a blue print for the vectors from the considered eigenspace of the original tree. Moreover, its matching properties can be utilized to determine the eigenspace dimension.

For previous research on spectra and eigenvectors of trees, bipartite graphs and other related graph classes the reader is referred to [6–11]. The partitioning of graphs according to eigenvector structure has been studied before, but with different aims [12].

As an application of our decomposition technique, we settle the question of characterizing all trees whose eigenspaces admit *simply structured* bases, i.e. bases that only contain entries from the set $\{0, 1, -1\}$. The task of finding simple eigenspace bases is a rather new research topic. As a second application we rediscover and generalize a result concerned with tree pattern matrices that was published in [5]. This topic is closely related to the studies of acyclic matrices. Some references in this area of research are for example [13–16].

2. Basics and notation

In this paper we will only consider finite, loopless, simple graphs. We will introduce some initial notation and will state further definitions along the way.

Let G be a graph. The vertex set of G will be written as $V(G)$. Given a set $M \subseteq V(G)$, we denote by $G \setminus M$ the graph formed by removing the vertices of M and all their adjacent edges from G. When we talk of a *vertex bipartition* of a bipartite graph we mean a disjoint partition of its vertex set into two sets such that every edge of the graph runs from a vertex of the first set to a vertex of the second set.

The eigenvalues of a graph G with vertex set $V = \{v_1, \dots, v_n\}$ are the eigenvalues of its adjacency matrix $A = (a_{ij})$ which is defined by $a_{ij} = 1$ if v_i is adjacent to v_j and $a_{ij} = 0$, otherwise. Note that this eigenvalue definition is independent of the chosen vertex order. Eigenvalues of graphs are real. For a bipartite graph λ is an eigenvalue if and only if $-\lambda$ is an eigenvalue of the graph as well [1]. Note that we do not consider the null vector an eigenvector although it formally belongs to an eigenspace.

Suppose that $Ax = \lambda x$, where $x = (x_1, \dots, x_n)^{\mathrm{T}}$. If we assign value x_i to vertex v_i, then it is easily seen that for every vertex the sum over the values of its neighbors equals λ times its own value. We will hereafter refer to this as the *summation rule*.

We conclude this section by quoting a basic result that we will frequently refer to:

Lemma 1 [13]. *Let T be a tree. Let v be an eigenvector of T for eigenvalue λ. If v does not have any zero entries, then λ necessarily has multiplicity one.*

3. Main results

3.1. Tree eigenvector decomposition

Let G be a graph and $M = \{X_1, \dots, X_r\}$ a set of mutually vertex disjoint subgraphs of G. Then by$G/\{X_i\}_{i=1}^{r}$ or G/M we denote the graph that results from the contraction of each subgraph X_i in G to a single vertex x_i. Further, let $\mathfrak{C}(G)$ denote the set of components of G.

Let x be an eigenvector for eigenvalue λ of graph G. Let $N_\lambda(G, x)$ be the set of those vertices of G on which x vanishes. Moreover, let $N_\lambda(G)$ mean the set of vertices on which every eigenvector for eigenvalue λ of G vanishes.

Lemma 2. *Let G be a graph and x an eigenvector for its eigenvalue λ. Then*:

1. *For any $C \in \mathfrak{C}(G \setminus N_\lambda(G, x))$, the restriction $x|_C$ is an eigenvector of the graph C for eigenvalue λ. If G is a tree, then $x|_C$ constitutes an eigenspace basis of the subtree C for eigenvalue λ.*
2. *For any $C \in \mathfrak{C}(G \setminus N_\lambda(G))$ the restriction $x|_C$ is either the null vector or an eigenvector of the graph C for eigenvalue λ. If G is a tree and $x|_C \neq 0$, then $x|_C$ does not contain any zero entries and, moreover, constitutes an eigenspace basis of the subtree C for eigenvalue λ.*

Proof. In the first case the claim follows directly from the definition of $N_\lambda(G, x)$, the summation rule and Lemma 1. The case $C \in \mathfrak{C}(G \setminus N_\lambda(G))$ is similar, with only one additional argument. Let $v_1, \ldots, v_k$ be the vertices of C. For every vertex v_i there exists an eigenvector x_i of T for eigenvalue λ whose restriction $x_i|_C$ does not vanish on v_i. It is straightforward to show (see e.g. Lemma 7 in [5]) that there exists a linear combination of these vectors x_i that has no zero entries so that by Lemma 1 the associated eigenvalue λ of C has multiplicity one. □

Let x be an eigenvector for eigenvalue λ of a given tree T. Further let C_i, $i = 1, \ldots, r$, be the elements of $\mathfrak{C}(T \setminus N_\lambda(T, x))$. We will now concentrate on a particularly interesting subset of $N_\lambda(T, x)$. Namely, let $N_\lambda^C(T, x)$ consist of all those vertices of $N_\lambda(T, x)$ that are adjacent to at least one of the subgraphs C_i in T.

Lemma 3. *Let T be a tree and x an eigenvector for its eigenvalue λ. Let C_i, $i = 1, \ldots, r$, be the elements of $\mathfrak{C}(T \setminus N_\lambda(T, x))$. Further let c_i denote the associated contracted vertices of $T/\{C_i\}_{i=1}^r$.*

Then the vertex set $N_\lambda^C(T, x) \cup \{c_1, \ldots, c_r\}$ induces a forest F in $T/\{C_i\}_{i=1}^r$ such that the leaves of F form a subset of $\{c_1, \ldots, c_r\}$ and are also leaves of $T/\{C_i\}_{i=1}^r$.

Proof. Clearly, the contraction $T/\{C_i\}_{i=1}^r$ of the tree T by the sub-forest $\bigcup\{C_i\}$ is a tree. So the induced subgraph F of $T/\{C_i\}_{i=1}^r$ must be a forest.

Now, consider an element v of $N_\lambda^C(T, x)$. By construction and since T is a tree there exists a one-to-one mapping of the non-zero weight neighbors of v to a subset of $\mathfrak{C}(T \setminus N_\lambda(T, x))$. By definition, v is adjacent to at least one component C_i, but since the sum over the neighbors of v must vanish we see that it must be adjacent to at least two such components. Consequently, v is adjacent to at least two of the vertices c_i in both $T/\{C_i\}_{i=1}^r$ and F. So the leaves in F are a subset of $\{c_1, \ldots, c_r\}$.

Assume that c_k is a leaf of F that is not a leaf of $T/\{C_i\}_{i=1}^r$. Then in $T/\{C_i\}_{i=1}^r$, there would exist a neighbor w of c_k such that $w \in N_\lambda(T, x) \setminus N_\lambda^C(T, x)$. But then w could only be adjacent to zero-weight vertices, a contradiction. □

In [3,4] graphs with nullity one and corresponding eigenvector without zero entries, so-called nut graphs, are studied. Nut graphs have a number of interesting properties. Clearly, the components of $T \setminus N_\lambda(T, x)$ are nut graphs if x is an eigenvector for eigenvalue 0. However, the theory

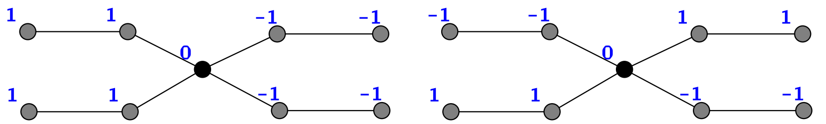

Fig. 1. Eigenvectors with the same x-skeleton.

on nut graphs does not yield any insight in the case of trees because it is easy to see that for a tree K_1 is the only possible nut graph.

In the following, let $S_\lambda(T, x)$ denote the forest F by Lemma 3 associated with a given tree T and eigenvector x. We call $S_\lambda(T, x)$ the x-*skeleton* of T.

Note that x-skeletons do not characterize an eigenspace basis, i.e. there may exist linearly independent eigenvectors x, x' for eigenvalue λ of a tree T such that $\mathfrak{C}(T \setminus N_\lambda(T, x)) = \mathfrak{C}(T \setminus N_\lambda(T, x'))$. An example is shown in Fig. 1 for $\lambda = 1$.

Theorem 4. *Let T be a tree and x an eigenvector for eigenvalue λ of T. Then,* $\mathfrak{C}(T \setminus N_\lambda(T, x)) \subseteq \mathfrak{C}(T \setminus N_\lambda(T))$.

Proof. Let $C \in \mathfrak{C}(T \setminus N_\lambda(T, x))$. Clearly, none of the vertices of C belong to the set $N_\lambda(T)$. Therefore C is a subgraph of some component $C' \in \mathfrak{C}(T \setminus N_\lambda(T))$. According to Lemma 2 the vector $x|_{C'}$ is an eigenvector for eigenvalue λ on C' and does not have any zero entries on C'. Hence $C = C'$. □

Corollary 5. *Let x, x' be eigenvectors for eigenvalue λ of a given tree and let $C \in \mathfrak{C}(T \setminus N_\lambda(T, x))$, $C' \in \mathfrak{C}(T \setminus N_\lambda(T, x'))$. Then either C and C' are identical or they are disjoint subgraphs of T.*

Corollary 6. *Let T be a tree with eigenvector x for eigenvalue λ. Then,*

$$N_\lambda^C(T, x) \subseteq N_\lambda(T).$$

Corollary 7. *Let T be a tree with eigenvalue λ. Then,*

$$\mathfrak{C}(T \setminus N_\lambda(T)) = \bigcup_x \mathfrak{C}(T \setminus N_\lambda(T, x)),$$

where the union is taken over all eigenvectors x for eigenvalue λ of T.

As a consequence of Corollary 7 we can safely merge the x-skeleton forests of an entire eigenspace. Let T be a tree and let $C_1, \ldots, C_r$ be the elements of $\mathfrak{C}(T \setminus N_\lambda(T))$. Let the associated contracted vertices in $T/\{C_i\}_{i=1}^r$ be $c_1, \ldots, c_r$. Denote the union of the sets $N_\lambda^C(T, x)$ by $N_\lambda^C(T)$. Now, we define the *skeleton* $S_\lambda(T)$ as the sub-forest of $T/\{C_i\}_{i=1}^r$ induced by the vertices of $N_\lambda^C(T) \cup \{c_1, \ldots, c_r\}$.

In Fig. 2 an example of a tree T with threefold eigenvalue 2 is shown along with its skeleton forest $S_2(T)$. The black vertices of T denote the vertices on which the respective eigenvector vanishes. It can be clearly seen how the respective components of $T \setminus N_\lambda(T, x)$ correspond to a part of the skeleton. The black vertices in the skeleton correspond to the set $N_2^C(T)$.

Lemma 8. *Let T be a tree with eigenvalue λ. Then $\mathfrak{C}(T \setminus N_\lambda^C(T))$ can be partitioned into $\mathfrak{C}(T \setminus N_\lambda(T))$ and a set of trees without eigenvalue λ.*

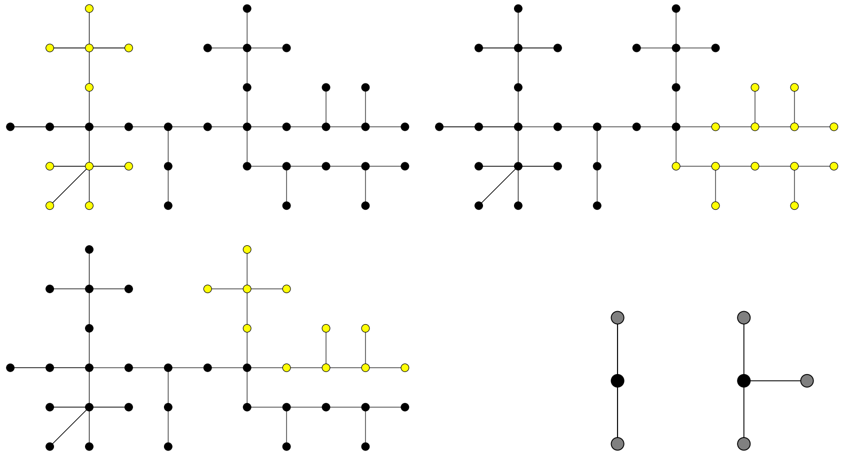

Fig. 2. Eigenvector zero-nonzero patterns of a tree and corresponding skeleton forest.

Proof. Considered as a subgraph of T, every component of $T \setminus N_\lambda(T)$ is adjacent only to vertices from $N_\lambda^C(T)$, but by definition does not contain such vertices. So $\mathfrak{C}(T \setminus N_\lambda(T)) \subseteq \mathfrak{C}(T \setminus N_\lambda^C(T))$. By construction all elements of $\mathfrak{C}(T \setminus N_\lambda(T))$ have eigenvalue λ. Now, let $C \in \mathfrak{C}(T \setminus N_\lambda^C(T)) \setminus \mathfrak{C}(T \setminus N_\lambda(T))$. All vertices of C necessarily belong to the set $N_\lambda(T)$ so that every eigenvector of T for eigenvalue λ must vanish on C.

Assume that there exists an eigenvector y of C for eigenvalue λ. Construct an eigenvector z for eigenvalue λ of T as follows. Firstly, set $z|_C = y$. Consider a vertex w that is adjacent to C in T and let v be the neighbor of w in C. Let ν be the value of y on v.

Case $\nu = 0$: simply set z to zero on the vertices of the particular component of $T \setminus C$ that contains w.

Case $\nu \neq 0$: clearly, $w \in N_\lambda^C(T)$ so that by construction, w has a neighbor $u \neq v$ that belongs to a component of $T \setminus N_\lambda(T)$ (since v does not). There exists an eigenvector x of T for eigenvalue λ that vanishes on C and w but does not vanish on u. We may assume w.l.o.g. that x has value $-\nu$ on u. Let T_u be the branch of T connected to w via u. Let T_F be the union of the branches connected to w via the neighbors of w different from u, v. Note that T_F is nonempty since x must fulfil the summation rule at vertex w. Set $z|_{T_F} = 0$ and $z|_{T_u} = x|_{T_u}$. Now, the summation rule holds for w and all the vertices of T_u and T_F.

Apply the described procedure for every eligible vertex w. After that the values of z are completely determined. This yields a valid eigenvector for eigenvalue λ of T that does not vanish on C, a contradiction. □

Combining Lemma 8 with Corollary 7 and Lemma 2 we can derive the following useful statement:

Lemma 9. *Let T be a tree and x an eigenvector for eigenvalue λ of T. Then for every $C \in \mathfrak{C}(T \setminus N_\lambda^C(T))$ the restriction $x|_C$ either has only zero entries or only non-zero entries. In the latter case it constitutes an eigenspace basis of the subgraph C of T.*

Observe that every vector from the null space of some x-skeleton can be trivially extended to a vector from the null space of the corresponding skeleton $S_\lambda(T)$.

Lemma 10. *Let T be a tree with eigenvalue λ. Further let $S' = T/\mathfrak{C}(T \setminus N_\lambda^C(T))$ and $S = S_\lambda(T)$. Then the skeleton S forms an induced sub-forest of the tree S' such that $S' \setminus V(S)$ contains no edges.*

Proof. Assume that S does not form an induced subgraph of S'. Then two vertices of S are adjacent in S' but not already in S. Since these vertices by construction must lie in the same component of S, the additional edge would create a cycle in S', which is impossible. By construction the vertices of $S' \setminus V(S)$ are mutually non-adjacent in S'. □

Lemma 10 allows us to derive the notion of a *meta skeleton* in which the components of the skeleton forest of a tree T with eigenvalue λ are joined by exactly those vertices contracted from the component trees of $\mathfrak{C}(T \setminus N_\lambda^C(T))$ that do not have eigenvalue λ (cf. Lemma 8).

Next we explore the relation between eigenspace bases of trees and null space bases of the respective skeleton forests.

Construction 11. Let $B = \{b_1, \ldots, b_r\}$ be an eigenspace basis for eigenvalue λ of a given tree T. Construct a basis $B' = \{b'_1, \ldots, b'_r\}$ of the same eigenspace as follows. Let initially $b'_i = b_i$ for $i = 1, \ldots, r$ and let $M = \emptyset$. There exists a component $C_1 \notin M$ of $T \setminus N_\lambda(T)$ such that $b_1|_{C_1}$ does not vanish. By Lemma 9 we can subtract suitable multiples of b'_1 from $b'_2, \ldots, b'_r$ such that $b'_i|_{C_1} = 0$ for $i = 2, \ldots, r$. Add C_1 to the set M. Proceed iteratively for b_j, $j = 2, \ldots, r$, by in turn finding a suitable $C_j \notin M$ and establishing $b'_i|_{C_j} = 0$ for $i = j + 1, \ldots, r$.

The previous construction immediately gives rise to the following observation.

Observation 12. Let T be a tree and let λ be an eigenvalue of T with multiplicity $r \geqslant 1$. Then, $|\mathfrak{C}(T \setminus N_\lambda(T))| \geqslant r$.

We say that a set $\{x_1, \ldots, x_r\}$ of eigenvectors for eigenvalue λ of a tree T is *straight* if the components of $T \setminus N_\lambda(T)$ can be numbered $C_1, \ldots, C_s$ such that for $j = 1, \ldots, r$ we have $x_j|_{C_j} \neq 0$ but $x_j|_{C_i} = 0$ for $i = j + 1, \ldots, r$. Observation 12 guarantees that $s \geqslant r$. Note that by Lemma 9 each condition $x_j|_{C_j} \neq 0$ actually means that x_j vanishes on none of the vertices of C_j. By Construction 11 every tree eigenspace has a straight basis.

Observation 13. Every straight set of tree eigenvectors is linearly independent.

Theorem 14. *Let T be a tree with eigenvalue λ and corresponding eigenspace basis B. Then for every vector $b \in B$ there exists a vector b' from the null space of the skeleton $S_\lambda(T)$ such that b' is non-zero exactly on the vertices corresponding to the contracted subgraphs of T on which its associated vector $b \in B$ does not vanish. If B is straight, then the vectors created from B are linearly independent.*

Proof. Let $b \in B$ and initialize $b' = 0$. In the following let $C(v)$ denote the contracted subgraph corresponding to a vertex v of $S_\lambda(T) \setminus N_\lambda^C(T)$. Moreover, if two vertices from $S_\lambda(T) \setminus N_\lambda^C(T)$ have a common neighbor in $S_\lambda(T)$ (necessarily from $N_\lambda^C(T)$) they are called *brothers*.

For every component S of $S_\lambda(T)$ proceed as follows. Fix a vertex s of $S \setminus N_\lambda^C(T)$. If b is non-zero on $C(s)$, then set b' to 1 on s. Consider s as visited and all other vertices of $S \setminus N_\lambda^C(T)$

as unvisited. We now employ a tree search that starts at s and iteratively corrects the values of b' on the vertices of $S \setminus N_\lambda^C(T)$ such that, finally, $b'|_S$ belongs to the null space of S and assumes the desired zero–nonzero pattern. The search only visits unvisited brothers of already visited vertices.

Let v be a visited vertex of $S \setminus N_\lambda^C(T)$ that has unvisited brothers. Mark all brothers of v as visited once the steps described below have been carried out. Let $W \subseteq N_\lambda^C(T)$ contain all vertices that are adjacent (in $S_\lambda(T)$) both to v and some unvisited brother of v. Now, iterate over the vertices $w \in W$. Let $v_1, \ldots, v_r$ be all those unvisited brothers of v that are adjacent to w and for which b does not vanish on $C(v_i)$. By construction, each vertex v_i has exactly one visited brother, namely v. Observe at this point that we have necessarily $r \geqslant 1$ if b does not vanish on $C(v)$ because else the summation rule would fail for b on the vertex in T that corresponds to w. Hence, it is always possible to assign suitable non-zero values to the vertices $v_1, \ldots, v_r$ such that b' fulfils the summation rule for vertex w.

By construction and the definition of a skeleton it follows immediately that b' is a valid eigenvector from the null space of $S_\lambda(T)$. Its zero-nonzero pattern is as claimed. If B is straight, then the set of vectors created from all the vectors of B using the above procedure is straight as well. Therefore it is linearly independent by Observation 13. □

Since every tree eigenspace has a straight basis we can immediately relate the dimensions of a tree eigenspace and the null space of the associated skeleton:

Corollary 15. *Let T be a tree with eigenvalue λ of multiplicity $r \geqslant 1$. Let s be the nullity of $S_\lambda(T)$. Then $r \leqslant s$.*

Theorem 16. *Let T be a tree with eigenvalue λ and let B' be a basis of the null space of its skeleton $S_\lambda(T)$. Then for every vector $b' \in B'$ there exists an eigenvector b of T for eigenvalue λ such that b is non-zero exactly on those subgraphs of T that correspond to vertices of $S_\lambda(T)$ on which b' does not vanish. If B' is straight, then the vectors created from B' are linearly independent.*

Proof. In view of Lemma 9 it is possible to use a technique similar to the one used in the proof of Theorem 14, just in the opposite direction. □

Corollary 17. *Let T be a tree with eigenvalue λ of multiplicity $r \geqslant 1$. Let s be the nullity of $S_\lambda(T)$. Then $r \geqslant s$.*

By Corollaries 15 and 17 we see that the multiplicity of the eigenvalue λ of a tree T equals the nullity of the skeleton $S_\lambda(T)$. It is well known that the nullity of a forest is closely linked to its matching properties. We will exploit these ties with respect to skeletons. But first let us generally relate maximum matchings of trees to eigenvectors of their null spaces. Maximum matchings of trees can be quite elegantly obtained using specialized algorithms [9,17].

Theorem 18. *Let T be a tree with edge set E. Let K contain all vertices of T that may be missed by some maximum matching of T. Further, let N contain all vertices of T that are saturated by all maximum matchings of T. Consider a fixed maximum matching M of T and let $K_M \subseteq K$ be the vertices missed by M.*

Then a simply structured null space basis of T can be constructed as follows. Pick a vertex $v \in K_M$ and find the subtree S_v of T formed by the union of all maximal paths that start at v and alternatingly contain edges from $E \setminus M$ and M, such that each edge in the path is incident to one vertex from N and one from $K \setminus (K_M \setminus \{v\})$. Assign weight 1 to all vertices of S_v whose distance to v is divisible by four, assign weight -1 if the distance is two modulo four, and assign zero to all other vertices of T.

Proof. Let us first verify that the summation rule holds on the tree S_v. By construction, the vertices of S_v receive non-zero weights if and only if they belong to $K \setminus (K_M \setminus \{v\})$, whereas the zero weight vertices of S_v all belong to the set N. Let w be a vertex of S_v. If $w \in K \setminus (K_M \setminus \{v\})$, then w has only neighbors belonging to the set N, so that the summation rule is trivial to check. If $w \in N$, then all its neighbors are from $K \setminus (K_M \setminus \{v\})$. However, w has necessarily degree 2 in S_v (cf. [17]). The two neighbors of w in S_v have values 1 and -1 so that the summation rule holds for w.

In order to verify the summation rule on T we only need to assert that no vertex w of S_v that belongs to $K \setminus (K_M \setminus \{v\})$ has a neighbor x in T that does not belong to S_v. Assume to the contrary that such vertices w, x exist. Now, x would either belong to K_M, in which case an M-augmenting path from v to x would exist in T and therefore contradict the maximality of M. Or there would exist an edge $xy \in M$ with $y \neq w$, contradicting the construction of S_v.

Linear independence of the constructed vectors is obvious by construction. That indeed a basis is formed follows from the fact that the rank of a tree equals twice the number of edges in a maximum matching of the tree (see e.g. [6,9]). □

Corollary 19. *Let T be a tree. Then the set of vertices saturated by all maximum matchings of T is exactly the set of vertices on which every vector from the null space of T vanishes.*

Corollary 20. *Let T be a tree and let R be the set of those vertices of T on which the null space of T does not completely vanish. Then the nullity of T equals the number of connected components of the subgraph of T induced by the set R minus the number of vertices of T that are adjacent to R but not contained in it.*

We will revisit Corollary 20 later on in Section 4.2.

Theorem 21. *Let T be a tree with eigenvalue λ.*

Then the set of vertices of the skeleton $S_\lambda(T)$ that may be missed by a maximum matching of the skeleton consists exactly of the vertices corresponding to the contracted components of $T \setminus N_\lambda(T)$.

The number of vertices of $S_\lambda(T)$ that are missed by a maximum matching of the skeleton equals the multiplicity of eigenvalue λ of T.

The non-zero entries of a vector from the null space of $S_\lambda(T)$ only occur on vertices that correspond to the contracted elements of $\mathfrak{C}(T \setminus N_\lambda(T))$.

Proof. This follows from Corollary 15, Corollary 17, Theorem 18 and Corollary 19. □

Concluding this section, let us remark without proof that a skeleton is its own eigenvalue 0 skeleton. In this sense, the skeleton construction cannot be arbitrarily iterated.

4. Applications

4.1. Simply structured tree eigenspace bases

In this section we give a characterization of trees for which simply structured eigenspace bases exist. It is easy to see that the only feasible eigenvalues that allow the construction of such bases are 0, 1, −1. Simply apply the summation rule to a leaf with non-zero value. It follows by a straightforward argument that such a leaf exists for every non-null eigenvector.

It has already been independently shown in [18,17] that every tree has such a simply structured basis for eigenvalue 0. We complete the characterization by investigating the other two possible eigenvalues. To this purpose we make use of the concept of decomposing trees by the zero entries of their eigenvectors that was presented earlier. Since trees are bipartite it now suffices to restrict further investigations to the eigenvalue 1. Given an eigenspace basis for eigenvalue 1 an eigenspace basis for eigenvalue −1 is readily obtained by negating the signs of all vector entries corresponding to the vertices of one part of the vertex bipartition.

Examples for eigenvectors for eigenvalue 1 that cannot be scaled to {0, 1, −1} entries can be found quite easily. See Fig. 3, where the claim follows by Lemma 1. In the following we will therefore attempt to characterize those trees that have a simply structured eigenspace basis for eigenvalue 1. A simple example of a tree with this property is the path P_5.

Assume that a tree with a simply structured eigenspace basis for eigenvalue 1 is decomposed according to the always-zero entries. Clearly, each such generated component has a single eigenvalue 1 and a corresponding eigenvector without zero entries, namely a {1, −1} vector. Since such eigenvectors are the building blocks for the composition of trees with simply structured bases for eigenvalue 1 we now direct our attention to them. It turns out that trees with {1, −1} eigenvector for single eigenvalue 1 can be characterized in a very elegant way.

Observation 22. Let x be an eigenvector for eigenvalue 1 of a given tree T. Then the value of x on a leaf equals the value on its unique neighbor.

Theorem 23. *A tree has a* {1, −1} *eigenvector for eigenvalue 1 if and only if the tree can be reduced to a* K_2 *graph by repeatedly selecting a subgraph as in Fig.* 4 *(where the vertices* u_0, u_1, w *must be leaves in the current reduced graph) and removing all its vertices except* z *from the current reduced graph.*

Proof. Let T be a tree with {1, −1} eigenvector x for eigenvalue 1. Clearly, T must have at least two vertices. If T is a complete graph K_2 there is nothing to show. So we may assume that T has at least three vertices.

Recall that the eccentricity of a vertex is its distance from the graph center and that the center of a tree consists of either a single vertex or a pair of adjacent vertices. Let u_0 be a leaf of T that has maximum eccentricity and v its only neighbor. Among those neighbors of v different from u_0 let z be that vertex which is closest to the center of T. Let $u_1, \ldots, u_r$ be the other neighbors

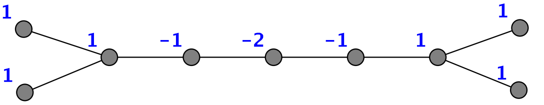

Fig. 3. Graph without {0,1,−1} eigenvector for eigenvalue 1.

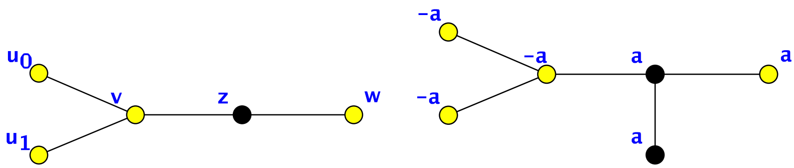

Fig. 4. Reduction subgraph and weights for {1,−1} eigenvectors.

of v besides u_0 and z. Since u_0 has maximum eccentricity the vertices $u_1, \ldots, u_r$ must also be leaves of T.

We may assume that v is not the sole center vertex of T. Otherwise T would be a star graph $K_{1,r+2}$, which does not have eigenvalue 1. Let w.l.o.g. x have value 1 on u_0. Then by Observation 22, x assumes the same value also on the vertices $u_1, \ldots, u_r, v$. The summation rule for vertex v requires a negative value of x on z. Therefore, $r = 1$ and x has value -1 on z.

We now claim that z is adjacent to a leaf with value -1. By the summation rule there exist at least two neighbors of z on which x assumes the value -1. Among these neighbors there exists at least one vertex w such that the branch adjacent to z via the edge wz does not contain any center vertices of T. Assume that w is not a leaf of T. Then by the summation rule w would have at least one neighbor w' with value 1. Again by the summation rule w' would have at least one neighbor w'' with value 1. But by our assumption about the location of the center of T the eccentricity of w'' is clearly greater than that of u_0, a contradiction.

Remove the vertices u_0, u_1, v, w from T. Clearly, T remains a tree. Moreover, the summation rule remains valid for all remaining vertices, in particular for z. Since z has at least one remaining neighbor it follows that T has at least two vertices. We can therefore iterate the reduction step until a graph K_2 has been obtained. The reduction procedure can also be applied for every subgraph of T isomorphic to the one in Fig. 4 if only u_0, u_1, w are leaves. The maximum eccentricity criterion only asserts the existence of a subtree suitable for reduction.

Conversely, assume that a tree can be decomposed in the described manner. Then we can assemble it from K_2 by iteratively selecting a vertex z and adding vertices u_0, u_1, z, w according to Fig. 4. The all ones vector forms an eigenspace basis for eigenvalue 1 of the graph K_2. After the addition of the vertices u_0, u_1, z, w we can uniquely augment the previous eigenvector to become a $\{1, -1\}$ eigenvector for eigenvalue 1 of the extended graph. The values on the newly added vertices depend only on the existing eigenvector value on z, cf. Fig. 4. Iterating this argument we find that T has a $\{1, -1\}$ eigenvector for eigenvalue 1. □

Corollary 24. *There exists a tree with n vertices that has a* $\{1, -1\}$ *eigenvector for eigenvalue 1 if and only if* $n \equiv 2 \bmod 4$.

In the following, let C denote the class of all trees with {1,−1} eigenvector for eigenvalue 1. Note that if a tree has a {1,−1} eigenvector for eigenvalue 1, then by Lemma 1, the eigenvalue 1 has necessarily multiplicity one.

Having investigated trees with {1,−1} eigenvectors it is now straightforward to achieve a characterization of trees with simply structured eigenspace bases for eigenvalue 1:

Theorem 25. *Let* T *be a tree with eigenvalue* 1. *Then there exists a simply structured basis for the corresponding eigenspace if and only if* $C \in \mathsf{C}$ *for every component* $C \in \mathfrak{C}(T \setminus N_1(T))$.

Proof. Necessity follows from Lemma 9. For sufficiency consider the reconstruction of (linearly independent) eigenvectors of T from the zero-nonzero patterns of a straight null space basis of its skeleton forest. Simply assign valid $\{1,-1\}$ eigenvectors to all contracted subgraphs of T where the chosen skeleton null space eigenvector is nonzero on the corresponding skeleton vertices. A valid eigenvector is obtained by establishing the summation rule for all vertices of $N_1^C(T)$. This can be achieved by conducting a breadth first search from a fixed nonzero skeleton vertex v. Each time a vertex of $N_1^C(T)$ is visited the summation rule for its partner vertex in T is enforced by suitably multiplying the values on the branches leading away from v. Since the branches have only values from the set $\{0,1,-1\}$ the only factors that are needed are 1 and -1 so that finally a $\{0,1,-1\}$ eigenvector is created. □

In theory, Theorem 25 provides us with a completely structural characterization of all trees whose eigenspace for eigenvalue 1 admits a simply structured basis. The class C is characterized by a reduction property and the set $N_1(T)$ is independent of the choice of a particular eigenspace basis so that essentially it is an intrinsic structural property of a tree as well.

4.2. Tree pattern matrices

Let M be a real $n \times n$ matrix. We define a (directed) graph $\Gamma(M)$ with vertices $v_1, \ldots, v_n$ such that there is an edge from v_i to v_j if and only if M has a non-zero entry at position (i, j). If $\Gamma(M)$ is a tree, then we call M a *tree pattern matrix*. Let $\operatorname{supp}(M; \lambda)$ denote the set of vertices of $\Gamma(M)$ on which the eigenspace for eigenvalue λ of M does not entirely vanish. We call this set the *support* of M with respect to λ. For a graph G, $\operatorname{supp}(G; \lambda)$ denotes the support of its adjacency matrix. Note that it is easy to find examples such that $\operatorname{supp}(M; \lambda)$ and $\operatorname{supp}(\Gamma(M); \lambda)$ are different.

We can extend Corollary 20 to the following result which has already been published in [5] but proven differently:

Theorem 26. *Let M be an $n \times n$ tree pattern matrix. Then the nullity of M equals the number of connected components of the subgraph of $\Gamma(M)$ induced by* $\operatorname{supp}(M; 0)$ *minus the number of vertices of $\Gamma(M)$ that are adjacent to* $\operatorname{supp}(M; 0)$ *but do not belong to this set.*

Proof. Let M be a tree pattern matrix and let A be the adjacency matrix of $\Gamma(M)$. Theorem 18 states that $\operatorname{supp}(A; 0)$ forms an independent vertex set in $\Gamma(M)$. Given a vector v from the null space of A we can transform it to a vector v' from the null space of M having the same zero-nonzero pattern as follows. Assign v to the vertices of $\Gamma(M)$. Conduct a breadth first search on $\Gamma(M)$ from a fixed vertex s and enforce new summation rules. To be precise, for every vertex z (as traversed by the breadth first search) it is possible to multiply each of its adjacent branches leading away from s with a nonzero factor such that the summation rule given by the line of M that corresponds to z holds. From a straight basis of the null space of A we can thus obtain a straight linearly independent set of vertices from the null space of M. A similar conversion can be employed for the opposite direction. Therefore, $\operatorname{supp}(M; 0) = \operatorname{supp}(A; 0) = \operatorname{supp}(\Gamma(M); 0)$. Now the result follows by Corollary 20. □

In fact, the results from the previous sections allow us to generalize even further. We quoted Lemma 1 only as a special case of what is actually proven in [13]. It has been shown that every eigenvector of a tree pattern matrix necessarily belongs to an eigenvalue with multiplicity one if it has no zero entries. Moreover, for the application of the summation rule none of the proofs given in Section 3 explicitly relied on the fact that it was induced by the adjacency matrix of the tree. Every row of a tree pattern matrix M induces a particular summation rule for the associated vertex of $\Gamma(M)$. The only difference to the summation rule used for the adjacency matrix is that for every vertex certain non-zero factors are applied to the weights of the neighbors before adding them up. Consequently, we can generalize the entire theory presented in Section 3 to cover eigenvectors of tree pattern matrices. In particular we obtain the following generalization of Theorem 26:

Theorem 27. *Let M be an $n \times n$ tree pattern matrix with eigenvalue λ. Then the dimension of the eigenspace of M for eigenvalue λ equals the number of connected components of the subgraph of $\Gamma(M)$ induced by $\mathrm{supp}(M;\lambda)$ minus the number of vertices of $\Gamma(M)$ that are adjacent to $\mathrm{supp}(M;\lambda)$ but do not belong to this set.*

One other noteworthy generalization is that eigenspace dimensions of tree patterned matrices are determined by sizes of maximum matchings of the respective associated skeletons.

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