

On spectral properties for graph matching and graph isomorphism problems

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Problems related to graph matching and isomorphisms are very important both from a theoretical and practical perspective, with applications ranging from image and video analysis to biological and biomedical problems. The graph matching problem is challenging from a computational point of view, and therefore different relaxations are commonly used. Although common relaxations techniques tend to work well for matching perfectly isomorphic graphs, it is not yet fully understood under which conditions the relaxed problem is guaranteed to obtain the correct answer. In this paper, we prove that the graph matching problem and its most common convex relaxation, where the matching domain of permutation matrices is substituted with its convex hull of doubly-stochastic matrices, are equivalent for a certain class of graphs, such equivalence being based on spectral properties of the corresponding adjacency matrices. We also derive results about the automorphism group of a graph, and provide fundamental spectral properties of the adjacency matrix.

Keywords: graph matching problem, convex relaxation, graph isomorphism problem, spectral properties.

1. Introduction

The theoretical and computational aspects behind graph isomorphisms and graph matching have been a great challenge for the scientific community for a long time. Maybe the easiest problem to state from this category is the graph isomorphism problem, which consists in determining whether two given graphs are isomorphic or not, that is, if there exists a bijection between the vertex sets of the graphs, preserving the edge structure. Besides the theoretical analysis, the graph isomorphism problem is also very interesting from the computational complexity point of view, since its complexity class is still unsolved: it is one of the few problems in NP not yet classified as P nor NP-complete [3].

The concept of graph automorphism, and its related properties, is closely connected to the graph isomorphism problem. An automorphism of a graph is a mapping from its vertex set onto itself, preserving the connectivity structure. The set of automorphisms forms a group under the composition operation. Of course, the identity map is always an automorphism, and when this is the only element in the group, we say that the graph has a trivial automorphism group. From the computational complexity point of view, computing the automorphism group is at least as difficult as solving the graph isomorphism problem.

The last problem we wish to discuss here is the so-called graph matching problem, which consists in finding an isomorphism between two graphs, and it is therefore harder than the graph isomorphism problem. Specifically, let G_A and G_B be two graphs with n vertices, and let \mathbf{A} and \mathbf{B} be their corresponding adjacency matrices. A common statement of the graph matching problem is to find the correspondence

between the nodes of G_A and G_B which minimizes some matching error. In terms of the corresponding adjacency matrices \mathbf{A} and \mathbf{B} , which encode the graph connectivity, this corresponds to finding a matrix \mathbf{P} in the set of permutation matrices \mathcal{P} , such that it minimizes a given distance between \mathbf{A} and $\mathbf{P}\mathbf{B}\mathbf{P}^\top$. A common choice is the Frobenius norm $\|\mathbf{A} - \mathbf{P}\mathbf{B}\mathbf{P}^\top\|_F^2$, and then the graph matching problem can be formally stated as

$$\min_{\mathbf{P} \in \mathcal{P}} \|\mathbf{A} - \mathbf{P}\mathbf{B}\mathbf{P}^\top\|_F^2 = \min_{\mathbf{P} \in \mathcal{P}} \|\mathbf{A}\mathbf{P} - \mathbf{P}\mathbf{B}\|_F^2. \quad (P_1)$$

Although polynomial algorithms have been developed for a few special types of graphs, like trees or planar graphs for example [3], the combinatorial nature of the permutation search makes this problem NP in general. As such, there are several and diverse techniques addressing the graph matching problem, including spectral methods [11] and relaxations techniques [6,12,13].

In this paper, we focus on a particular and very common relaxation technique, which consists in relaxing the feasible set (the set of permutation matrices) to its convex hull. By virtue of the Birkhoff–von Neuman theorem, the convex hull of \mathcal{P} is the set of doubly stochastic matrices $\mathcal{D} = \{\mathbf{M} \in \mathbb{R}^{n \times n} : \mathbf{M}_{ij} \geq 0, \mathbf{M}\mathbf{1} = \mathbf{1}, \mathbf{M}^\top \mathbf{1} = \mathbf{1}\}$, that is, the set of matrices with non-negative entries such that each row and column sum up to one.

The relaxed version of the problem is then

$$\hat{\mathbf{P}} = \arg \min_{\mathbf{P} \in \mathcal{D}} \|\mathbf{A}\mathbf{P} - \mathbf{P}\mathbf{B}\|_F^2, \quad (P_2)$$

which is a convex problem. However, the resulting $\hat{\mathbf{P}}$ is a doubly stochastic matrix and not necessarily a permutation matrix, or in general the solution to (P_1) .

Indeed, since the feasible set of problem (P_2) is the convex hull of the feasible set of problem (P_1) , every solution of the first problem is also a solution of the relaxed graph matching problem. A very important question is under which hypothesis the solution set of these two problems (P_1) and (P_2) coincide. It is easy to see that, if there are two permutation matrices that solve the graph matching problem, then every matrix on the straight line joining them is a solution of problem (P_2) , since this problem is convex. Therefore, the least that one should ask for these two problems to be equivalent is for the solution of (P_1) to be unique. When the two graphs are isomorphic, this is equivalent to asking for the automorphism group of the graphs to be the trivial group.

The relaxation to doubly stochastic matrices is closely related to the concept of *fractional isomorphism* [10]. We say that two graphs G_A and G_B are *fractionally isomorphic* when there exist a doubly stochastic matrix $\hat{\mathbf{P}}$ such that $\mathbf{A}\hat{\mathbf{P}} = \hat{\mathbf{P}}\mathbf{B}$. The chapter about fractional isomorphism in [10] provides a great introduction to the subject, including the relationship with graph isomorphism.

A probabilistic analysis of the equivalence between the original and the relaxed graph matching problems is provided in [9]. Basically, the authors prove that, when two graphs are correlated (but not necessarily isomorphic), then the unique solution of a non-convex relaxation is almost always the correct permutation matrix; while, on the other hand, the underlying alignment is almost always not a solution of the commonly used convex relaxation, where the permutation set is replaced by the doubly-stochastic set as above.

On the other hand, in [1] the authors prove the equivalence of the original graph matching problem and a relaxed version for a particular kind of graphs which they call *friendly*, based on spectral properties. In this work, we extend these results, proving the (deterministic) equivalence for a larger set of graphs, and also shedding light on some new spectral graph properties.

2. Main result

In this section, we consider two isomorphic graphs G_A and G_B with n vertices each, and adjacency matrices \mathbf{A} and \mathbf{B} , respectively. Let $\mathbf{P}_0 \in \mathcal{P}$ be the permutation matrix associated to the isomorphism between the two graphs, that is, $\mathbf{B} = \mathbf{P}_0 \mathbf{A} \mathbf{P}_0^\top$.

Since the graphs considered here are isomorphic, then the minimum (either over \mathcal{D} or \mathcal{P}) of $\|\mathbf{A}\mathbf{P} - \mathbf{P}\mathbf{B}\|_F^2$ is zero, and it is achieved (at least) at \mathbf{P}_0 . Both problems can then be re-stated as solving the set of linear equations $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{B}$ over $\mathbf{P} \in \mathcal{P}$ or $\mathbf{P} \in \mathcal{D}$.

Now, consider that by the simple change of variables $\mathbf{Q} = \mathbf{P}\mathbf{P}_0$. Then for any solution \mathbf{P} to the relaxed problem (P_2), it holds that

$$\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{B} \iff \mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{P}_0\mathbf{A}\mathbf{P}_0^\top \iff \mathbf{A}\mathbf{P}\mathbf{P}_0 = \mathbf{P}\mathbf{P}_0\mathbf{A} \iff \mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}. \quad (2.1)$$

Note that the change of variables is a multiplication by a permutation matrix, and hence the set of doubly stochastic matrices is invariant under this mapping. Therefore, any solution to $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}$ over $\mathbf{Q} \in \mathcal{D}$ leads, via the change of variables, to a solution of $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{B}$ with $\mathbf{P} \in \mathcal{D}$. This allows us to state the equivalency between both problems (P_1) and (P_2) using only one of the adjacency matrices. Specifically, the problem $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}$ with $\mathbf{Q} \in \mathcal{D}$ has a trivial solution $\mathbf{Q} = \mathbf{I}$, which corresponds to the solution \mathbf{P}_0 of the problem $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{B}$ with $\mathbf{P} \in \mathcal{D}$. Then the matrix \mathbf{P}_0 will be the unique solution of problem (P_2) if and only if the identity is the unique solution of $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}$ with $\mathbf{Q} \in \mathcal{D}$.

Now, since \mathbf{A} is a symmetric matrix, we can consider its spectral decomposition $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$, where \mathbf{D} is a diagonal matrix containing the eigenvalues and \mathbf{U} is an orthonormal matrix containing the eigenvectors as columns, denoted as u_i , for $i = 1 \dots n$.

The main result of [1] states that if \mathbf{A} has no repeated eigenvalues, and no eigenvector u_i is perpendicular to the vector of ones $\mathbf{1}$, then problems (P_1) and (P_2) are equivalent. This is illustrated in Fig. 1, where some graph properties are represented. Here *asymmetric* means that the automorphism group of the graph is trivial, *simple spectrum* means that the adjacency matrix has no repeated eigenvalues, *non-orthogonal to $\mathbf{1}$* means that no eigenvector u_i verifies $u_i^\top \mathbf{1} = 0$, and the *regular circle* contains regular graphs, i.e. graphs such that each vertex has the same number of neighbors. The intersection of *simple spectrum* and *non-orthogonal to $\mathbf{1}$* graphs is what the authors of [1] call *friendly* graphs, and they prove the equivalence of problems (P_1) and (P_2) for this class.

As observed above, a necessary condition for problems (P_1) and (P_2) to be equivalent, is for the automorphism group of the graph to be the trivial group. However, this condition is not sufficient. Take for instance a regular graph, and denote by \mathbf{J} the barycenter of the set of doubly stochastic matrices, $\mathbf{J} = (1/n)\mathbf{1}\mathbf{1}^\top$. Hence, it is very easy to see that, if \mathbf{A} is the adjacency matrix of a regular graph, then $\mathbf{A}\mathbf{J} = \mathbf{J}\mathbf{A}$. Therefore, there is a solution to problem (P_2) which is not a permutation matrix. Since there are regular graphs with a trivial automorphism group (like the Frucht graph [7] for instance), then this condition cannot be sufficient. In Fig. 1, this is represented with the small red circle, which intersects both the asymmetric and simple spectrum sets (see Section 4 for examples of graphs in each intersection). In summary, we can hope for problems (P_1) and (P_2) to be equivalent inside the *asymmetric* set minus the regular graphs. So far, we know from [1] that this is true for *friendly* graphs, being this until now the largest known class for which the relaxation is equivalent to the original problem.

The next theorems extend the set where these problems are equivalent to a larger set of graphs. Theorem 2.2 is stronger than Theorem 2.1, but we include both proofs for the sake of clarity, since both have pedagogic value.

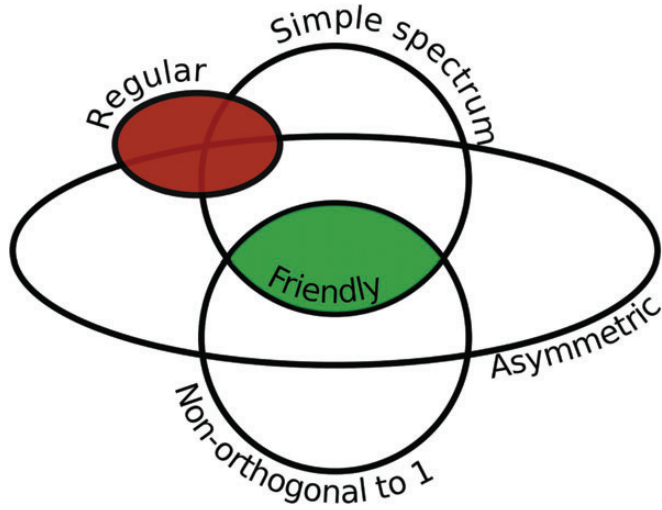


FIG. 1. Graph classes and equivalence of problems (P_1) and (P_2) . Graphs with trivial automorphism group are represented in the *asymmetric* set (we know that graphs for which (P_1) and (P_2) are equivalent are inside this set), graphs whose adjacency matrices have no repeated eigenvalues are represented as the *simple spectrum* set, *non-orthogonal to 1* means that no eigenvector u_i verifies $u_i^\top \mathbf{1} = 0$, and the *regular* circle contains regular graphs. Graphs in the intersection of *simple spectrum* and *non-orthogonal to 1* are called *friendly* graphs, and here the equivalence of problems (P_1) and (P_2) holds [1]. These problems are not equivalent for regular graphs. A key question addressed in this work is how far we can extend the green zone of equivalence inside the asymmetric set.

THEOREM 2.1 If \mathbf{A} has no repeated eigenvalues (simple spectrum), and there are k eigenvectors u_i such that $u_i^\top \mathbf{1} = 0$, each one of these vectors having at least $2k + 1$ non-zero entries, then problems (P_1) and (P_2) are equivalent.

Proof. We want to prove that the identity is the unique solution to the problem $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}$ for $\mathbf{Q} \in \mathcal{D}$. Let us write the equality $\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A}$ in terms of the eigenvector decomposition of \mathbf{A} :

$$\mathbf{A}\mathbf{Q} = \mathbf{Q}\mathbf{A} \Leftrightarrow \mathbf{U}\mathbf{D}\mathbf{U}^\top \mathbf{Q} = \mathbf{Q}\mathbf{U}\mathbf{D}\mathbf{U}^\top \Leftrightarrow \mathbf{U}^\top \mathbf{U}\mathbf{D}\mathbf{U}^\top \mathbf{Q}\mathbf{U} = \mathbf{U}^\top \mathbf{Q}\mathbf{U}\mathbf{D}\mathbf{U}^\top \mathbf{U} \Leftrightarrow \mathbf{D}\mathbf{U}^\top \mathbf{Q}\mathbf{U} = \mathbf{U}^\top \mathbf{Q}\mathbf{U}\mathbf{D}.$$

Now, let us denote by \mathbf{F} the new unknown matrix $\mathbf{F} = \mathbf{U}^\top \mathbf{Q}\mathbf{U}$. The problem can now be stated as

$$\mathbf{D}\mathbf{F} = \mathbf{F}\mathbf{D}, \quad \mathbf{U}\mathbf{F}\mathbf{U}^\top \in \mathcal{D}, \quad (P_F)$$

and we now want to prove that $\mathbf{F} = \mathbf{I}$ is the unique solution of this last problem.

It is easy to see that, since \mathbf{D} is diagonal with no repeated entries in the diagonal, then \mathbf{F} has to be diagonal as well in order to commute with \mathbf{D} .

Let us write the conditions for $\mathbf{U}\mathbf{F}\mathbf{U}^\top$ to be in \mathcal{D} :

$$(c1) \quad \mathbf{U}\mathbf{F}\mathbf{U}^\top \mathbf{1} = \mathbf{1},$$

$$(c2) \quad \mathbf{U}\mathbf{F}^\top \mathbf{U}^\top \mathbf{1} = \mathbf{1},$$

$$(c3) \quad (\mathbf{U}\mathbf{F}\mathbf{U}^\top)_{ij} \geq 0 \quad \forall i, j.$$

Since \mathbf{F} is diagonal, and in particular $\mathbf{F} = \mathbf{F}^\top$, then the first two conditions are redundant, and one of them can be eliminated. Left-multiplying the first condition by \mathbf{U}^\top , we obtain $\mathbf{F}\mathbf{U}^\top\mathbf{1} = \mathbf{U}^\top\mathbf{1}$, and calling $\mathbf{v} = \mathbf{U}^\top\mathbf{1}$, condition (c1) can be written as $\mathbf{F}\mathbf{v} = \mathbf{v}$.

Without loss of generality, we can assume that the k eigenvectors u_i satisfying $u_i^\top\mathbf{1} = 0$ are the first k columns in \mathbf{U} . Therefore, $\mathbf{v}_i = 0$ for $i = 1 \dots k$, and $\mathbf{v}_i \neq 0$ for $i = k + 1 \dots n$. As \mathbf{F} is diagonal, the equations $\mathbf{F}\mathbf{v} = \mathbf{v}$ can be easily written as $\mathbf{F}_{i,i}\mathbf{v}_i = \mathbf{v}_i$. When $\mathbf{v}_i \neq 0$, the only way for this equation to hold is when $\mathbf{F}_{i,i} = 1$. This means that $\mathbf{F}_{i,i} = 1$ for $i = k + 1 \dots n$, and this is sufficient to guarantee that the first two conditions hold.

For analyzing the third condition, let us decompose the matrix product assuming that \mathbf{F} is a diagonal matrix with $\mathbf{F}_{i,i} = 1$ for $i = k + 1 \dots n$:

$$\mathbf{U}\mathbf{F}\mathbf{U}^\top = \sum_{i=1}^n u_i \mathbf{F}_{i,i} u_i^\top = \sum_{i=1}^k u_i \mathbf{F}_{i,i} u_i^\top + \sum_{i=k+1}^n u_i u_i^\top.$$

We can now add and subtract $\sum_{i=1}^k u_i u_i^\top$, leading to

$$\mathbf{U}\mathbf{F}\mathbf{U}^\top = \sum_{i=1}^k u_i (\mathbf{F}_{i,i} - 1) u_i^\top + \sum_{i=1}^n u_i u_i^\top = \mathbf{I} + \sum_{i=1}^k u_i (\mathbf{F}_{i,i} - 1) u_i^\top.$$

Let us denote by $\mathbf{L} = \sum_{i=1}^k (1 - \mathbf{F}_{i,i}) u_i u_i^\top$, and therefore $\mathbf{U}\mathbf{F}\mathbf{U}^\top = \mathbf{I} - \mathbf{L}$.

Observe that the matrix \mathbf{L} satisfies $\mathbf{L}\mathbf{1} = \mathbf{0}$, since every vector u_i participating in the sum satisfies $u_i^\top\mathbf{1} = 0$; and note also that all the elements in the diagonal are $\mathbf{L}_{j,j} \geq 0$, otherwise the corresponding entry of $\mathbf{U}\mathbf{F}\mathbf{U}^\top$ would be $(\mathbf{U}\mathbf{F}\mathbf{U}^\top)_{j,j} > 1$, violating the doubly stochastic condition.

Now, let us assume that there is a solution \mathbf{F} to problem (P_F) different from the identity, and let us analyze the corresponding \mathbf{L} matrix trying to find a contradiction. The condition (c3) dictates that $(\mathbf{I} - \mathbf{L})_{i,j} \geq 0$ for all i, j , therefore the \mathbf{L} matrix has no positive elements off the diagonal. On the other hand, since \mathbf{F} is diagonal and we have assumed $\mathbf{F} \neq \mathbf{I}$, then at least one of the values $\mathbf{F}_{i,i}$ ($i \leq k$) is different from 1. The corresponding eigenvector u_i , which has at least $2k + 1$ non-zero elements by hypothesis, will be actually used in the summation constructing \mathbf{L} , and therefore this guarantees that at least $2k + 1$ elements in the diagonal of \mathbf{L} are strictly positive.

Considering then the following just described properties for the \mathbf{L} matrix:

- $\mathbf{L}\mathbf{1} = \mathbf{0}$,
- $\mathbf{L}_{i,j} \leq 0$ for all $i \neq j$,
- $\mathbf{L}_{i,i} \geq 0$ for all $i = 1 \dots n$,
- $\mathbf{L} = \mathbf{L}^\top$,

we can associate an undirected graph G_L such that \mathbf{L} is its Laplacian matrix.¹ Moreover, since at least $2k + 1$ diagonal elements of \mathbf{L} are non-zero (and strictly positive), at least $2k + 1$ elements off the diagonal are non-zero (and strictly negative), since each row has to add up to zero.

Now, each off diagonal element of the Laplacian matrix \mathbf{L} corresponds to an edge of the graph G_L . Since the matrix \mathbf{L} is symmetric, the graph G_L is undirected, and each edge appears twice in the

¹ Given a graph with adjacency matrix \mathbf{M} , its Laplacian matrix is defined as $\mathbf{L} = \mathbf{S} - \mathbf{M}$, where \mathbf{S} is the degree matrix, i.e. a matrix having the degree of each node in the corresponding diagonal element, and zeros elsewhere.

Laplacian matrix. Since there are at least $2k + 1$ non-zero elements off the diagonal of \mathbf{L} , the auxiliary graph G_L has at least $\lfloor (2k + 1)/2 \rfloor = k + 1$ edges. It is easy to see that, if the number of edges is $e \geq k + 1$, then the auxiliary graph G_L has at most $C \leq n - (k + 1)$ connected components.

Remembering that the number of connected components C is given by the multiplicity of the 0 eigenvalue of the Laplacian matrix \mathbf{L} , then the rank of \mathbf{L} has to be at least $\text{rank}(\mathbf{L}) = n - C \geq k + 1$.

However, by construction, \mathbf{L} is the sum of k rank-one matrices, and therefore $\text{rank}(\mathbf{L}) \leq k$, which is a contradiction. This proves that the only solution to problem (P_F) is the identity, concluding the proof of the theorem. \square

This proof, and therefore the class of equivalence between problems (P_1) and (P_2) , can be further extended by noting that we originally asked for every eigenvector orthogonal to $\mathbf{1}$ to have at least $2k + 1$ non-zero elements, but in the proof we only used this fact for one of these eigenvectors. It might be the case, for instance, that only one of the elements $\mathbf{F}_{i,i}$ is different from one, and therefore the matrix \mathbf{L} has rank one. In this case, it would be sufficient to ask for the corresponding eigenvector to have at least three non-zero elements. The problem is that we do not know in advance which or how many of the eigenvectors will be used in the summation to construct the \mathbf{L} matrix. However, it is possible to weaken the hypothesis as shown next.

Let us consider all the k eigenvectors satisfying $u_i^\top \mathbf{1} = 0$, and sort them according to the number of non-zero elements, such that $|u_1|_0 \leq |u_2|_0 \leq \dots \leq |u_k|_0$, where $|\cdot|_0$ is the ℓ_0 pseudo-norm, which counts the non-zero elements of a vector.

THEOREM 2.2 If \mathbf{A} has no repeated eigenvalues, and there are k eigenvectors u_i such that $u_i^\top \mathbf{1} = 0$, sorted as above and satisfying $|u_i|_0 \geq 2i + 1$, then problems (P_1) and (P_2) are equivalent.

Proof. This proof follows exactly the same procedure as the previous one, with minor changes.

Let us assume, as before, that there is a solution $\mathbf{F} \neq \mathbf{I}$ to problem (P_F) . In order to fulfill condition c1), the last $n - k$ diagonal elements of F have to be one, i.e. $\mathbf{F}_{i,i} = 1$ for $i = k + 1, \dots, n$. For the first k diagonal elements, there might be some 0 values. Let M be the greatest index of the eigenvectors actually used in the sum, meaning $M = \max\{i \in 1 \dots k : \mathbf{F}_{i,i} \neq 0\}$.

We can then write

$$\mathbf{L} = \sum_{i=1}^M (1 - \mathbf{F}_{i,i}) u_i u_i^\top.$$

Since $|u_M|_0 \geq 2M + 1$, the auxiliary graph G_L has at least $M + 1$ edges. Therefore the number of connected components satisfies $C \leq n - (M + 1)$, and hence $\text{rank}(\mathbf{L}) \geq M + 1$. The contradiction, as before, comes from the fact that \mathbf{L} is the sum of M rank one matrices, concluding the proof. \square

As noted above, a necessary condition for the problems (P_1) and (P_2) to be equivalent is for the automorphism group of G_A to be the trivial group. Therefore, we have the following corollary.

COROLLARY 2.1 If \mathbf{A} has no repeated eigenvalues, and there are k eigenvectors u_i such that $u_i^\top \mathbf{1} = 0$, sorted according to their ℓ_0 norm as above, and satisfying $|u_i|_0 \geq 2i + 1$, then the automorphism group of the corresponding graph G_A is the trivial group.

3. Interpretation and additional results

It is clear that the spectral decomposition of an adjacency matrix provides a lot of information about the automorphism group of a graph, and the graph matching problem itself. However, very little is known

about how the eigenvalues and eigenvectors of the adjacency matrix affect the graph properties (a brief but very interesting analysis is given in [4]). In this section, we discuss some links between these two fields, paying particular attention to the equivalence of problems (P_1) and (P_2) , and also discussing more general novel properties.

As noted in the previous section, asymmetry of a graph is a necessary condition for problems (P_1) and (P_2) to be equivalent, although is not sufficient, with asymmetric regular graphs serving as counter-examples (see red region in Fig. 1). It is interesting to note that regular graphs have the vector $\mathbf{1}$ as an eigenvector, and since the adjacency matrix is symmetric, its eigenvectors are orthogonal to each other, therefore there are $n - 1$ eigenvectors satisfying $u_i^\top \mathbf{1} = 0$. Hence, the condition asked in [1] is violated not only by one eigenvector, but by $n - 1$ of them.

Besides this observation, it is not clear the interpretation of the non-existence of eigenvectors perpendicular to $\mathbf{1}$.

Let us focus now on the properties of eigenvectors orthogonal to $\mathbf{1}$ with restricted support, as in the statement of Theorem 2.1.

3.1 The simplest case: one single eigenvector u such that $u^\top \mathbf{1} = 0$

Let us assume here that \mathbf{A} is the adjacency matrix of a graph G_A with no repeated eigenvalues and only one eigenvector u satisfying $u^\top \mathbf{1} = 0$. Now, if this vector u has strictly more than two non-zero entries, i.e. $|u|_0 > 2$, then this graph falls into the hypothesis of Theorem 2.1. Therefore, the graph has trivial automorphism group, and if G_B is an isomorphic graph, problems (P_1) and (P_2) are equivalent.

Since the sum of the entries of u is zero, the only remaining case is when u has exactly two non-zero elements. Assuming that the eigenvectors are normalized, the eigenvector u is of the form

$$u = \left(0, \dots, 0, \frac{1}{\sqrt{2}}, 0, \dots, 0, \frac{-1}{\sqrt{2}}, 0, \dots, 0 \right).$$

Let s and t be the indices of the non-zero coefficients. Since u is an eigenvector, then we have $\mathbf{A}u = \lambda u$. Now, denoting by \mathbf{A}_s and \mathbf{A}_t the columns of \mathbf{A} at positions s and t , respectively, and taking into account the particular structure of u , the product $\mathbf{A}u$ is simply the difference between these two columns: $\mathbf{A}u = \frac{1}{\sqrt{2}}(\mathbf{A}_s - \mathbf{A}_t) = \lambda u$. Therefore, columns \mathbf{A}_s and \mathbf{A}_t are identical, except for the coordinates s and t . This means that the nodes corresponding to indices s and t have exactly the same connectivity pattern with the rest of the nodes in the graph.

Consider now the rest of the involved entries (nodes). Let $\tilde{\mathbf{A}}$ be the 2×2 sub-matrix formed by entries (s, s) , (s, t) , (t, s) and (t, t) of matrix \mathbf{A} , and let $w = (\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$. We then have $\tilde{\mathbf{A}}w = \lambda w$. It is easy to see that, since the entries in $\tilde{\mathbf{A}}$ are either 1 or 0, then only three values of λ are possible: -1 , 0 and 1 , corresponding to the following situations:

- $\lambda = -1$: the matrix is $\tilde{\mathbf{A}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, therefore, nodes s and t are connected and they have no loops;
- $\lambda = 0$: the matrix is either $\tilde{\mathbf{A}} = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ or $\tilde{\mathbf{A}} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$. Therefore, nodes s and t are either connected and both have loops, or not connected without loops;
- $\lambda = 1$: the matrix is $\tilde{\mathbf{A}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, therefore, nodes s and t are not connected and both of them have loops.

As in the previous section, consider the eigen-decomposition $\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{U}^\top$, which transforms the problem $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{A}$ into $\mathbf{D}\mathbf{F} = \mathbf{F}\mathbf{D}$, where the new unknown matrix \mathbf{F} is defined as $\mathbf{F} = \mathbf{U}^\top\mathbf{P}\mathbf{U}$, or equivalently, $\mathbf{P} = \mathbf{U}\mathbf{F}\mathbf{U}^\top$. As before, since \mathbf{A} has no repeated eigenvalues, \mathbf{F} is necessarily diagonal, and therefore $\mathbf{P} = \mathbf{U}\mathbf{F}\mathbf{U}^\top$ is one possible eigen-decomposition of \mathbf{P} .

Now, the matrix \mathbf{U} of normalized eigenvectors of \mathbf{A} is unique, up to changes of sign in each column. This is not true for \mathbf{P} , since it has repeated eigenvalues. However, any orthogonal eigen-decomposition of \mathbf{P} can be obtained as an orthogonal transformation (rotation and/or symmetries) of \mathbf{U} .

Given that \mathbf{P} is block-diagonal, one possible eigen-decomposition can be obtained by combining the eigen-decompositions of each block. The lower part of \mathbf{P} is an identity block, and hence all eigenvalues are equal to 1, with canonical eigenvectors. The rest are 2×2 blocks with the following decomposition:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

Therefore, a plausible eigen-decomposition for \mathbf{P} is $\mathbf{P} = \mathbf{V}\mathbf{E}\mathbf{V}^\top$, with:

$$\mathbf{E} = \begin{pmatrix} -1 & & & & & & & & & \mathbf{0} \\ & 1 & & & & & & & & \\ & & \ddots & & & & & & & \\ & & & -1 & & & & & & \\ & & & & 1 & & & & & \\ & & & & & 1 & & & & \\ & & & & & & \ddots & & & \\ \mathbf{0} & & & & & & & & & 1 \end{pmatrix}, \quad \mathbf{V} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & & & & & & \mathbf{0} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & & & & & & \\ & & \ddots & & & & & & & \\ & & & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & & & \\ & & & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & & & & & \\ & & & & & 1 & & & & \\ & & & & & & \ddots & & & \\ \mathbf{0} & & & & & & & & & 1 \end{pmatrix}.$$

Since the columns of both \mathbf{U} and \mathbf{V} are a possible basis of the eigenvalues of \mathbf{P} , the matrix \mathbf{U} can be thought as an orthogonal transformation of \mathbf{V} that leaves invariant the eigenspaces S_{-1} and S_1 (eigenspaces of \mathbf{P} associated with eigenvalues -1 and 1 , respectively). Observe that the eigenspace S_{-1} is composed by vectors orthogonal to $\mathbf{1}$, and therefore, in the orthogonal transformation from \mathbf{V} to \mathbf{U} , the whole subspace S_{-1} will be mapped to a subspace orthogonal to $\mathbf{1}$. Let k be the dimension of the subspace S_{-1} , and let us denote by $\tilde{\mathbf{U}}$ the set of the k eigenvectors of \mathbf{A} (columns of \mathbf{U}) corresponding to the eigenspace S_{-1} after the linear mapping. These columns of \mathbf{U} , as argued above, are orthogonal to $\mathbf{1}$. Analogously, let $\tilde{\mathbf{V}}$ be formed by the columns of \mathbf{V} associated with the eigenvalue -1 , so the columns of $\tilde{\mathbf{V}}$ are a basis of S_{-1} .

Given that we assumed $\mathbf{P} \neq \mathbf{I}$, there is at least one 2×2 non-identity block like the one described above, and therefore $k \geq 1$. Since S_{-1} is invariant under the orthogonal transformation, then the mapping of this subspace can be written as linear combinations of the elements of the basis, this is, $\tilde{\mathbf{U}} = \tilde{\mathbf{V}}\mathbf{T}$,

where \mathbf{T} is an orthogonal matrix. Since, according to the previous description, $\tilde{\mathbf{V}}$ has the form

$$\tilde{\mathbf{V}} = \frac{1}{\sqrt{2}} \underbrace{\begin{pmatrix} -1 & 0 & \dots & 0 \\ 1 & 0 & \dots & 0 \\ 0 & -1 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & -1 \\ 0 & 0 & \dots & 1 \\ \vdots & \vdots & & \vdots \end{pmatrix}}_{k \text{ columns}},$$

then $\tilde{\mathbf{U}}$ is conformed by k vectors with $2k$ non-zero entries at most. Moreover, each one of these vectors has an even number of non-zero entries. \square

We have simulated millions of Erdős–Rényi graphs, and have obtained empirical evidence suggesting that there is always a subset of these k vectors formed by r vectors with exactly $2r$ non-zero entries each, in the same location, which correspond to the $2r$ nodes which are permuted in the automorphism (see examples in Section 4). However, the arguments used in the previous proof are not sufficient to formally prove this.

On the other hand, the empirical evidence also suggests that a converse of this last statement may be true. We formulate then the following conjecture.

CONJECTURE 3.1 If \mathbf{A} has no repeated eigenvalues, and there exist a set of r eigenvectors u_i satisfying $u_i^\top \mathbf{1} = 0$, each one of them with exactly $2r$ non-zero entries, in the same location, then the group of automorphisms of G_A is not trivial.

We know that this is true for $k = 1$, Section 3.1. The proof for the general case, as well as other relations between spectral properties and the automorphism group, are part of future work.

4. Graph examples

Figure 1 shows different sets of graphs according to the relevant characteristics for this paper, principally about eigenvectors and eigenvalues. For instance, the class of graphs where Theorems 2.1 and 2.2 apply lays on the intersection of asymmetric and simple spectrum graphs, but outside the *non-orthogonal to 1* set. It is important therefore to show that there exist graphs in this subset, and in general that each subset in the diagram is not empty.

As mentioned above, the Frucht graph [7], illustrated in Fig. 2 (left), serves as an example of regular graphs with trivial automorphism group and simple spectrum. The regular graph in Fig. 2 (right) also has trivial automorphism group, but the adjacency matrix has repeated eigenvalues.

The graph of Fig. 3 is an example of a graph with simple spectrum, but where there is an eigenvector u such that $u^\top \mathbf{1} = 0$, and therefore this is not a *friendly* graph. This eigenvector has four non-zero elements, and hence Theorem 2.1 applies. As a consequence, for any isomorphic graph, problems (P_1) and (P_2) are equivalent, and in particular the automorphism group of this graph is trivial. Since the graph is not *friendly*, the results of [1] do not hold for this graph.

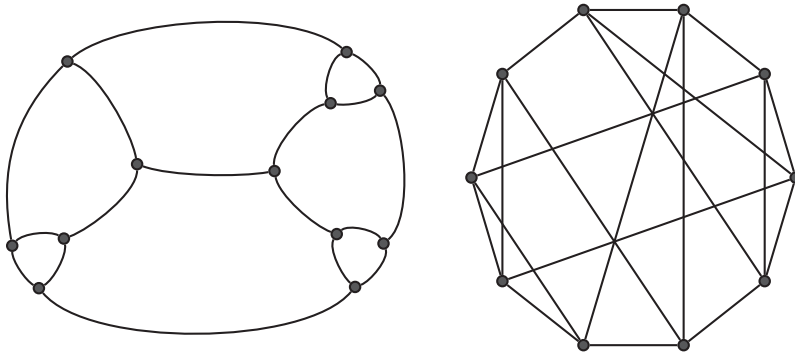


FIG. 2. Regular graphs with trivial automorphism group. Left: the Frucht graph, with simple spectrum. Right: a regular asymmetric graph with repeated eigenvalues.

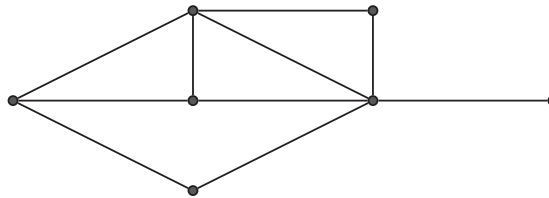


FIG. 3. A non-friendly graph, with simple spectrum but one eigenvector orthogonal to $\mathbf{1}$.

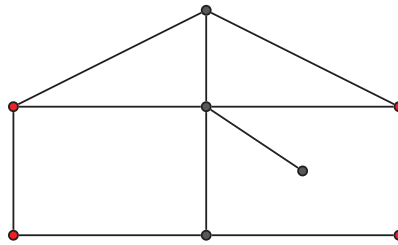


FIG. 4. A graph with simple spectrum but non-trivial automorphism group.

The graph in Fig. 4 has simple spectrum but non-trivial automorphism group. Indeed, it has two eigenvectors u_1 and u_2 orthogonal to $\mathbf{1}$, each one with four non-zero elements. Namely, the eigenvectors are

$$u_1 = \left(\frac{1}{2}, \frac{1}{2}, \frac{-1}{2}, \frac{-1}{2}, 0, 0, 0\right)$$

and

$$u_2 = \left(\frac{1}{2}, \frac{-1}{2}, \frac{1}{2}, \frac{-1}{2}, 0, 0, 0\right).$$

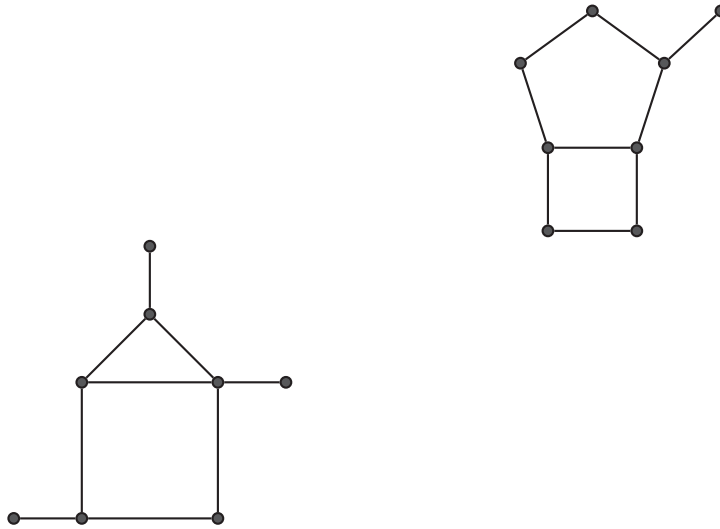


FIG. 5. Asymmetric graphs with repeated eigenvalues, with (left) and without (right) eigenvectors orthogonal to $\mathbf{1}$.

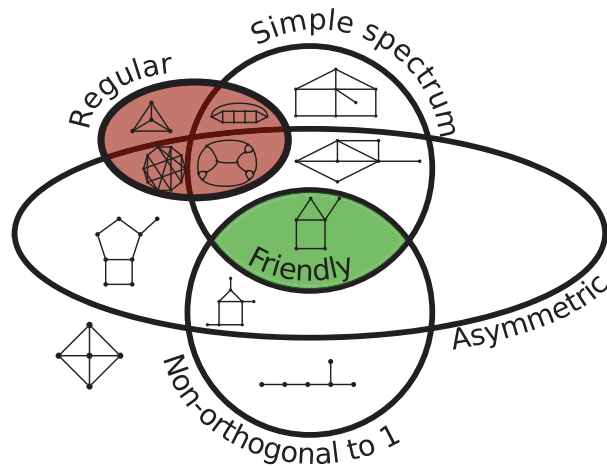


FIG. 6. Examples of graphs in each class.

Illustrating the Conjecture 3.1, the first four coordinates of the eigenvectors correspond to the four red nodes of the graph. The non-trivial automorphism consist on permuting the two lower nodes between themselves, and the two upper nodes between themselves, as it can be clearly seen in the figure. Of course, Theorems 2.1 and 2.2 do not apply for this graph.

The following two graphs, illustrated in Fig. 5, have trivial automorphism group and both have repeated eigenvalues. The first one has one eigenvector orthogonal to $\mathbf{1}$, while the second one has no eigenvector u satisfying $u^T \mathbf{1} = 0$.

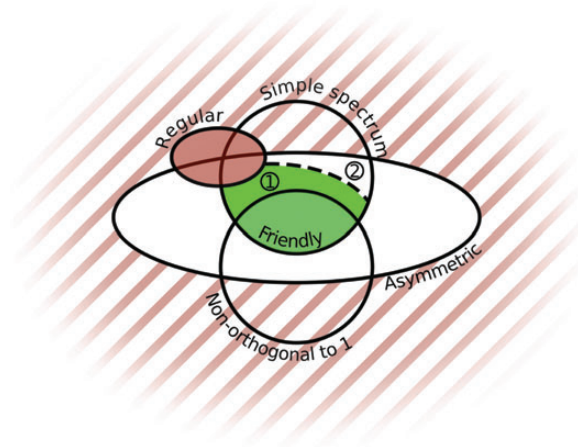


FIG. 7. Regions where problems (P_1) and (P_2) are known to be equivalent (green) and non-equivalent (red). Outside the *asymmetric* set and inside the *regular* set, the problems are known to be non-equivalent. Problems are equivalent for *friendly* graphs [1], and in the green zone 1 by virtue of the theorems proved in Section 2. The zone 2 consists of non-regular asymmetric graphs with simple spectrum, but not satisfying the conditions of Theorems 2.1 or 2.2; although this subset might be non-empty, since we could not find examples of graphs in this zone.

Finally, Fig. 6 shows the same diagram as in Fig. 1, but with examples of graphs inside each intersection, demonstrating that none of these subsets is empty.

5. Conclusion

We have addressed the equivalence of the graph matching problem with its most common convex relaxation, generalizing the results in [1], and extending the analysis to graph automorphism properties.

Theorem 2.1 and the stronger version, Theorem 2.2, state conditions on the spectral properties of the adjacency matrix of a graph in order for the graph matching problem and the convex relaxation to be equivalent. Specifically, if the adjacency matrix has simple spectrum, and the eigenvectors orthogonal to vector $\mathbf{1}$ have enough non-zero entries, then the equivalence between the two problems holds. This gives also a set of easily verifiable conditions implying that the automorphism group of a graph is trivial.

The extension of the set where problems (P_1) and (P_2) are known to be equivalent, due to these new results, is shown in Fig. 7.

In addition to the main theorems, we provided evidence that these particular eigenvectors, orthogonal to $\mathbf{1}$, contain critical information about the symmetries of the graph, specially in their non-zero entries.

During the last decades, important theory was developed on eigenvalues and eigenvectors of the Laplacian matrix of a graph, with very important theoretic results, which brought important applications. The new results here presented shed light on some spectral properties of the adjacency matrix, and leave open some other questions about the link between these properties and the automorphisms of the graph.

Finally, the relationship between the main results in this paper and the theory of fractional isomorphisms (in particular, with equitable partitions) is a very interesting topic, which is part of the future work.

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