Descriptive Complexity of Graph Spectra

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Abstract

Two graphs are cospectral if their respective adjacency matrices have the same multi-set of eigenvalues. A graph is said to be determined by its spectrum if all graphs that are cospectral with it are isomorphic to it. We consider these properties in relation to logical definability. We show that any pair of graphs that are elementarily equivalent with respect to the three-variable counting first-order logic C^3 are cospectral, and this is not the case with C^2, nor with any number of variables if we exclude counting quantifiers. We also show that the class of graphs that are determined by their spectra is definable in partial fixed-point logic with counting. We relate these properties to other algebraic and combinatorial problems.

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1. Introduction

The spectrum of a graph G is the multi-set of eigenvalues of its adjacency matrix. Even though it is defined in terms of the adjacency matrix of G, the spectrum does not, in fact, depend on the order in which the vertices of G are listed. In other words, isomorphic graphs have the same spectrum. The converse is false: two graphs may have the same spectrum without being isomorphic. We say that two graphs are cospectral if they have the same spectrum.

The spectrum of graphs is a graph invariant and forms the basis for some approaches to testing graph isomorphism. There are polynomial time tests that will distinguish graphs that are not cospectral. And cospectral, non-isomorphic graphs tend to be harder to distinguish—the best graph isomorphism testing algorithms tend to perform poorly on these. Attempts have been made to extend the techniques by considering the spectra of matrices other than the adjacency matrix, associated with graphs. So far, none of these provide a complete isomorphism test.

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Our aim in this paper is to study the relationship of cospectrality as an equivalence relation on graphs in relation to a number of other approximations of isomorphism coming from logic, combinatorics and algebra. We also investigate the definability of cospectrality and related notions in logic.

Specifically, we show that for any graph G, we can construct a formula ϕ_G of first-order logic with counting, using only three variables (*i.e.* the logic C^3) so that $H \models \phi_G$ only if H is cospectral with G. From this, it follows that elementary equivalence in C^3 refines cospectrality, a result that also follows from [1]. In contrast, we show that cospectrality is incomparable with elementary equivalence in C^2, or with elementary equivalence in L^k (first-order logic with k variables but without counting quantifiers) for any k. We show that on strongly regular graphs, cospectrality exactly coincides with C^3-equivalence.

For definability results, we show that cospectrality of a pair of graphs is definable in FPC, inflationary fixed-point logic with counting. We also consider the property of a graph G to be *determined by its spectrum*, meaning that all graphs cospectral with G are isomorphic with G. We establish that this property is definable in *partial fixed-point logic with counting* (PFPC).

In section 2, we say some words motivating this work and construct some basic first-order formulas that we use to prove various results later, and we also review some well-known facts in the study of graph spectra. In section 3, we make explicit the connection between the spectrum of a graph and the total number of closed walks on it. Then we discuss aspects of the class of graphs that are uniquely determined by their spectra. Also, we show a lower bound for the distinguishability of graph spectra in the finite-variable logic.

In section 4, we give an overview of a combinatorial algorithm for distinguishing between non-isomorphic graphs, and study the relationship with other algorithms of algebraic and combinatorial nature. We note that something expected happens for strongly regular graphs, which are graphs with high combinatorial regularity. In section 5, we establish some results about the logical definability of cospectrality and of the property of being a graph determined by its spectrum. We end by making some concluding remarks in section 6.

2. Preliminaries

Our motivation comes from spectral graph theory:

Conjecture 1 ([2])**.** *Almost every graph is determined by its spectrum.*

Background material on this conjecture can be found in [2, 3, 4, 5] and the reference contained therein. In this document, we will consider graphs determined by their spectra in relation to logical definability. We would like to approach the above conjecture via logical definability. As we shall see in Proposition 2, graphs elementary equivalent with respect to the counting logic C^3 are necessarily cospectral. Indeed their complements are as well cospectral (Corollary 1). This just follows from the fact that if a C^3-formula distinguishes G from H, then the same formula with $\neg E$ replacing E separates the complement of G from the complement of H.

We shall consider the first-order language of signature $\sigma = \{E\}$, where E is a binary relation symbol interpreted as an irreflexive symmetric binary relation called *adjacency*. Then a σ-structure $G = (V_G, E_G)$ is called a *simple undirected graph*. The universe V_G of G is called the *vertex set* and its elements are called *vertices*. The unordered pairs of vertices in the interpretation E_G of E are called *edges*. Formally, a *graph* is an element of the elementary class axiomatised by the first-order σ-sentence:

$$\forall x \forall y (\neg E(x,x) \wedge (E(x,y) \rightarrow E(y,x))).$$

The *adjacency matrix* of an n-vertex graph G with vertices $v_1, \ldots, v_n$ is the $n \times n$ matrix A_G with entry $(A_G)_{ij} = 1$ if vertex v_i is adjacent to vertex v_j, and $(A_G)_{ij} = 0$ otherwise. By definition, every adjacency matrix is real and symmetric with diagonal elements all equal to zero. A *permutation matrix* P is a binary matrix with a unique 1 in each row and column. Permutation matrices are orthogonal matrices so the inverse P^{-1} of P is equal to its transpose P^T. Two graphs G and H are *isomorphic* if there is a bijection h from V_G to V_H that preserves adjacency. The existence of such a map is denoted by $G \cong H$. From this definition it is not difficult to see that two graphs G and H are isomorphic if, and only if, there exists a permutation matrix P such that $P^T A_G P = A_H$.

The *characteristic polynomial* of an n-vertex graph G is a polynomial in a single variable λ defined as $p_G(\lambda) := \det(\lambda I - A_G)$, where $\det(\cdot)$ is the operation of computing the determinant of the matrix inside the parentheses, and I is the identity matrix of the same order as A_G. The *spectrum* of G is the multi-set $\mathrm{sp}(G) := \{\lambda : p_G(\lambda) = 0\}$, where each root of $p_G(\lambda)$ is considered according to its multiplicity. If $\lambda \in \mathrm{sp}(G)$ then $\lambda I - A_G$ is not invertible, and so there exists a nonzero vector u such that $A_G u = \lambda u$. A vector like u is called an *eigenvector* of G corresponding to λ. The elements in $\mathrm{sp}(G)$ are called the *eigenvalues* of G. Two graphs are called *cospectral* if they have the same spectrum.

The *trace* of a matrix is the sum of all its diagonal elements. By the definition of matrix multiplication, for any two matrices A, B we have $\mathrm{tr}(AB) = \mathrm{tr}(BA)$, where $\mathrm{tr}(\cdot)$ is the operation of computing the trace of the matrix inside the parentheses. Therefore, if G and H are two isomorphic graphs then

$$\begin{aligned} \mathrm{tr}(A_H) &= \mathrm{tr}(P^T A_G P) \\ &= \mathrm{tr}(A_G P P^T) \\ &= \mathrm{tr}(A_G) \end{aligned}$$

and so, $\mathrm{tr}(A_G^k) = \mathrm{tr}(A_H^k)$ for any $k \geq 0$.

Suppose that A is an $n \times n$ matrix with (possibly repeated) eigenvalues $\lambda_1, \ldots, \lambda_n$. For each $0 \leq d \leq n$, the *elementary symmetric polynomial* e_d in the eigenvalues of A is defined as the sum of all distinct products of d distinct eigenvalues of A:

$$\begin{aligned}
e_0(\lambda_1, \dots, \lambda_n) &:= 1; \\
e_1(\lambda_1, \dots, \lambda_n) &:= \sum_{i=1}^{n} \lambda_i; \\
e_d(\lambda_1, \dots, \lambda_n) &:= \sum_{1 \le i_1 < \cdots < i_d \le n} \lambda_{i_1} \cdots \lambda_{i_d} \qquad\qquad \text{for } 1 < d \le n.
\end{aligned}$$

For $1 \le k \le n$, if $s_k(\lambda_1, \dots, \lambda_n) := \sum_{i=1}^{n} \lambda_i^k$ then the equation

$$e_k(\lambda_1, \dots, \lambda_n) = \frac{1}{k} \sum_{j=1}^{k} (-1)^{j-1} e_{k-j}(\lambda_1, \dots, \lambda_n) s_k(\lambda_1, \dots, \lambda_n)$$

is called the k-th *Newton's identity.*

The next result establishes the connection to be explored in the next section, between computing the spectrum of a graph and counting the number of closed walks that it contains.

Proposition 1. *For n-vertex graphs G and H, the following are equivalent:*

1. *G and H are cospectral;*
2. *G and H have the same characteristic polynomial;*
3. $\mathrm{tr}(A_G^k) = \mathrm{tr}(A_H^k)$ *for* $1 \le k \le n$.

Proof. By the spectral decomposition theorem, computing the trace of the k-th powers of a real symmetric matrix A will give the sum of the k-th powers of the eigenvalues of A. It is well-known that the elementary symmetric polynomials $e_0, e_1, \dots, e_n$ evaluated in the eigenvalues of A are the coefficients of the characteristic polynomial of A modulo a 1 or -1 factor. That is,

$$\begin{aligned}
\det(\lambda I - A) &= \prod_{i=1}^{n} (\lambda - \lambda_i) \\
&= \lambda^n - e_1(\lambda_1, \dots, \lambda_n)\lambda^{n-1} + \cdots + (-1)^n e_n(\lambda_1, \dots, \lambda_n) \\
&= \sum_{d=0}^{n} (-1)^{n+d} e_{n-d}(\lambda_1, \dots, \lambda_n) \lambda^d.
\end{aligned}$$

So if we know $\sum_{i=1}^{n} \lambda_i^k = \mathrm{tr}(A_G^k) = \mathrm{tr}(A_H^k)$ for $1 \le k \le n$, then using Newton's identities we can obtain all the symmetric polynomials in the eigenvalues, and so we can reconstruct the characteristic polynomial of A. Hence (3) implies (2). That (2) implies (1) is obvious, and (1) implies (3) is trivial. $\square$

3. Spectra and Walks

Given a graph G and a positive integer l, a *walk of length l* in G is a sequence $v_0, v_1, \dots, v_l$ of vertices of G, such that consecutive vertices are adjacent in G.

Formally, $v_0, v_1, \ldots, v_l$ is a walk of length l in G if, and only if, $\{v_{i-1}, v_i\} \in E_G$ for $1 \leq i \leq l$. We say that the walk $v_0, v_1, \ldots, v_l$ *starts* at v_0 and *ends* at v_l. A walk of length l is said to be *closed* (or *l-closed*, for short) if it starts and ends in the same vertex, *i.e.*, $v_0 = v_l$.

Since the ij-th entry of A_G^l is precisely the number of walks of length l in G starting at v_i and ending at v_j, by Proposition 1, we have that the spectrum of G is completely determined if we know the total number of closed walks for each length up to the number of vertices in G. Thus, two graphs G and H are cospectral if, and only if, the total number of l-closed walks in G is equal to the total number of l-closed walks in H for all $l \geq 0$.

For an example of cospectral non-isomorphic graphs, let $G = C_4 + K_1$ be the disjoint union of the 4-vertex cycle with a vertex, and $H = K_{1,4}$ the $(1, 4)$-complete bipartite graph. The spectrum of both G and H is the multi-set $\{-2, 0, 0, 0, 2\}$. However, G contains an isolated vertex while H is a connected graph.

3.1. Finite Variable Logics with Counting

For each positive integer k, let C^k denote the fragment of first-order logic in which only k distinct variables can be used but we allow *counting quantifiers*: so for each $i \geq 1$ we have a quantifier $\exists^i$ whose semantics is defined so that $\exists^i x\phi$ is true in a structure if there are at least i distinct elements that can be substituted for x to make ϕ true. We use the abbreviation $\exists^{=i} x\phi$ for the formula $\exists^i x\phi \wedge \neg\exists^{i+1} x\phi$ that asserts the existence of exactly i elements satisfying ϕ. We write $G \equiv^{C^k} H$ to denote that the graphs G and H are not distinguished by any formula of C^k. Note that C^k-*equivalence* is the usual first-order elementary equivalence relation restricted to formulas using at most k distinct variables and possibly using counting quantifiers.

We show that for integers k, l, with $k \geq 0$ and $l \geq 1$, there is a formula $\psi_k^l(x, y)$ of C^3 so that for any graph G and vertices $v, u \in V_G$, $G \models \psi_k^l[v, u]$ if, and only if, there are exactly k walks of length l in G that start at v and end at u. We define this formula by induction on l. Note that in the inductive definition, we refer to a formula $\psi_k^l(z, y)$. This is to be read as the formula $\psi_k^l(x, y)$ with all occurrences of x and z (free or bound) interchanged. In particular, the free variables of $\psi_k^l(x, y)$ are exactly x, y and those of $\psi_k^l(z, y)$ are exactly z, y.

For $l = 1$, the formulas are defined as follows:

$$\psi_0^1(x, y) := \neg E(x, y); \quad \psi_1^1(x, y) := E(x, y);$$
$$\text{and} \quad \psi_k^1(x, y) := \text{false} \quad \text{for} \quad k > 1.$$

For the inductive case, we first introduce some notation. We say that a collection $(i_1, k_1), \ldots, (i_r, k_r)$ of pairs of integers, with $i_j, k_j \geq 1$ is an *indexed partition* of k if the $k_1, \ldots, k_r$ are pairwise distinct and $k = \sum_{j=1}^r i_j k_j$. Let K denote the set of all indexed partitions of k and note that this is a finite set.

Now, assume we have defined the formulas $\psi_k^l(x, y)$ for all values of $k \geq 0$. We proceed to define them for $l + 1$:

$$\psi_0^{l+1}(x, y) := \forall z(E(x, z) \rightarrow \psi_0^l(z, y))$$

$$\psi_k^{l+1}(x,y) := \bigvee_{(i_1,k_1),\ldots,(i_r,k_r)\in K} \Big(\big(\bigwedge_{j=1}^{r} \exists^{=i_j} z\ \psi_{k_j}^{l}(z,y) \big) \wedge \exists^{d} z\ E(x,z) \Big),$$

where $d = \sum_{j=1}^{r} i_j$. We have used i_j to denote the number of neighbours of x for which there are exactly k_j walks of length l from each of them to y. Note that without allowing counting quantification it would be necessary to use many more distinct variables to rewrite the last formula.

Given an n-vertex graph G, as noted before $(A_G^l)_{ij}$ is equal to the number of walks of length l in G from vertex v_i to vertex v_j, so $(A_G^l)_{ij} = k$ if, and only if, $G \models \psi_k^l(v_i, v_j)$. Once again, let K denote the set of indexed partitions of k. For each integer $k \geq 0$ and $l \geq 0$, we define the sentence

$$\phi_k^l := \bigvee_{(i_1,k_1),\ldots,(i_r,k_r)\in K} \Big(\bigwedge_{j=1}^{r} \exists^{=i_j} x \exists y \big(x = y \wedge \psi_k^l(x,y) \big) \Big). \tag{1}$$

Then we have $G \models \phi_k^l$ if, and only if, the total number of closed walks of length l in G is exactly k. Hence $G \models \phi_k^l$ if, and only if, $\mathrm{tr}(A_G^l) = k$. Thus, we have the following proposition.

Proposition 2. *If $G \equiv^{C^3} H$ then G and H are cospectral.*

Proof. Suppose G and H are two non-cospectral graphs. Then there must be some positive integer l, such that $\mathrm{tr}(A_G^l) \neq \mathrm{tr}(A_H^l)$. Hence the total number of closed walks of length l in G is different from the total number of closed walks of length l in H (see Proposition 1). If k is the total number of closed walks of length l in G, then $G \models \phi_k^l$ and $H \not\models \phi_k^l$ with ϕ_k^l defined as (1). Since ϕ_k^l is a sentence of C^3, we conclude that $G \not\equiv^{C^3} H$ and the proposition follows. $\square$

For any n-vertex graph G and $l \geq 1$, there exists a positive integer k_l such that $\mathrm{tr}(A_G^l) = k_l$. Since having the traces of powers of the adjacency matrix of G up to the number of vertices is equivalent to having the spectrum of G, we can define a sentence

$$\phi_G := \bigwedge_{l=1}^{n} \phi_{k_l}^l \tag{2}$$

of C^3 such that for any graph H, we have $H \models \phi_G$ if, and only if, $\mathrm{sp}(G) = \mathrm{sp}(H)$. The complement $\bar{G}$ of a graph G is defined as the graph with vertex set V_G and adjacency matrix $J - I - A_G$, where J denotes the all-ones matrix. Thus, we can define a sentence $\phi_{\bar{G}}$ of C^3 with $\neg E$ replacing E in ϕ_G so that $\bar{H} \models \phi_{\bar{G}}$ if, and only if, $\mathrm{sp}(\bar{G}) = \mathrm{sp}(\bar{H})$.

Corollary 1. *Graphs that are elementary equivalent with respect to the counting logic C^3 are cospectral with cospectral complements.*

3.2. Graphs Determined by Their Spectra

The goal of this subsection and later of section 5 is to generalise in a syntactical way the property of being a graph uniquely determined by its spectrum.

We say that a graph G is *determined by its spectrum* (for short, DS) when for any graph H, if $\mathrm{sp}(G) = \mathrm{sp}(H)$ then $G \cong H$. In words, a graph is determined by its spectrum when it is the only graph up to isomorphism with a certain spectrum. In Proposition 2 we saw that C^3-equivalent graphs are necessarily cospectral. That is, if two graphs G and H are C^3-equivalent then G and H must have the same spectrum.

In general, determining whether a graph has the DS property (*i.e.*, the equivalence class induced by having the same spectrum coincides with its isomorphism class) is an open problem in spectral graph theory (see, *e.g.* [2]). Given a graph G and a positive integer k, we say that the logic C^k *identifies* G when for all graphs H, if $G \equiv^{C^k} H$ then $G \cong H$. Let $\mathcal{C}_n^k$ be the class of all n-vertex graphs that are identified by C^k. Since C^2-equivalence corresponds to indistinguishability by the 1-dimensional Weisfeiler-Lehman algorithm [6], from a classical result of Babai, Erdős and Selkow [7], it follows that $\mathcal{C}_n^2$ contains almost all n-vertex graphs. Let DS_n be the class of all DS n-vertex graphs.

The 1-dimensional Weisfeiler-Lehman algorithm (see Section 4) does not distinguish any pair of non-isomorphic regular graphs of the same degree with the same number of vertices. Hence, if a regular graph is not determined up to isomorphism by its number of vertices and its degree, then it is not in $\mathcal{C}_n^2$. However, there are regular graphs that are determined by their number of vertices and their degree. For instance, the complete graph on n vertices, which gives an example of a graph in $\mathrm{DS}_n \cap \mathcal{C}_n^2$.

Let T be a tree on n vertices. By a well-known result from Schwenk [8], with probability one there exists another tree T' such that T and T' are cospectral but not isomorphic. From a result of Immerman and Lander [6] we know that all trees are identified by C^2. Hence T is an example of a graph in $\mathcal{C}_n^2$ and not in DS. On the other hand, the disjoint union of two complete graphs with the same number of vertices is a graph which is determined by its spectrum. That is, $K_m + K_m$ is DS (see [2, Section 6.1]). For each $m > 2$ it is possible to construct a connected regular graph G_{2m} with the same number of vertices and the same degree as $K_m + K_m$. Hence G_{2m} and $K_m + K_m$ are not distinguishable in C^2 and clearly not isomorphic. This shows that cospectrality and elementary equivalence with respect to the two-variable counting logic is incomparable.

From a result of Babai and Kučera [9], we know that a graph randomly selected from the uniform distribution over the class of all unlabeled n-vertex graphs (which has size equal to $2^{n(n-1)/2}$) is not identified by C^2 with probability equal to $(o(1))^n$. Moreover, in [10] Kučera presented an efficient algorithm for labelling the vertices of random regular graphs from which it follows that the fraction of regular graphs which are not identified by C^3 tends to 0 as the number of vertices tends to infinity. Therefore, almost all regular n-vertex graphs are in $\mathcal{C}_n^3$. Summarising, DS_n and $\mathcal{C}_n^2$ overlap and both are contained in $\mathcal{C}_n^3$.

3.3. Lower Bounds

Having established that C^3-equivalence is a refinement of cospectrality, we now look at the relationship of the latter with equivalence in finite variable logics without counting quantifiers. First of all, we note that some cospectral graphs can be distinguished by a formula using just two variables and no counting quantifiers. Next, we show that counting quantifiers are essential to the argument from the previous section in that cospectrality is not subsumed by equivalence in any finite-variable fragment of first-order logic in the absence of such quantifiers.

Let L^k denote the fragment of first-order logic in which each formula has at most k distinct variables.

Proposition 3. *There exists a pair of cospectral graphs that can be distinguished in L^2.*

Proof. Let us consider the following two-variable first-order sentence:

$$\psi := \exists x \forall y \ \neg E(x, y).$$

For any graph G we have that $G \models \psi$ if, and only if, there is an isolated vertex in G. Hence $C_4 + K_1 \models \psi$ and $K_{1,4} \not\models \psi$. Therefore, $C_4 + K_1 \not\equiv^{L^2} K_{1,4}$. On the other hand, as noted at the beginning of this section, these two graphs are cospectral. □

For each $r, s \geq 0$, the *extension axiom* $\eta_{r,s}$ is the first-order sentence

$$\forall x_1 \ldots \forall x_{r+s} \Bigg(\bigg(\bigwedge_{i \neq j} x_i \neq x_j \bigg) \to \exists y \bigg(\bigwedge_{i \leq r} E(x_i, y) \wedge \bigwedge_{i > r} \neg E(x_i, y) \wedge x_i \neq y \bigg) \Bigg).$$

A graph G satisfies the *k-extension property* if $G \models \eta_{r,s}$ for all $r + s = k$. In [11] Kolaitis and Vardi proved that if two graphs G and H both satisfy the k-extension property, then there is no formula of L^k that can distinguish them. If this happens, we write $G \equiv^{L^k} H$. Fagin [12] proved that for each $k \geq 0$, almost all graphs satisfy the k-extension property. Hence almost all graphs are not distinguished by any formula of L^k.

Let q be a prime power such that $q \equiv 1 \pmod 4$. The *Paley graph* of order q is the graph $P(q)$ with vertex set $\mathbb{F}_q$, the finite field of order q, where two vertices i and j are adjacent if there is a positive integer x such that $x^2 \equiv (i - j) \pmod q$. Since $q \equiv 1 \pmod 4$ if, and only if, $x^2 \equiv -1 \pmod q$ is solvable, we have that -1 is a square in $\mathbb{F}_q$ and so, $(j - i)$ is a square if and only if $-(i - j)$ is a square. Therefore, adjacency in a Paley graph is a symmetric relation and so, $P(q)$ is undirected. Blass, Exoo and Harary [13] proved that if q is greater than $k^2 2^{4k}$, then $P(q)$ satisfies the k-extension property.

Now, let $q = p^r$ with p an odd prime, r a positive integer, and $q \equiv 1 \pmod 3$. The *cubic Paley graph* $P^3(q)$ is the graph whose vertices are elements of the finite field $\mathbb{F}_q$, where two vertices $i, j \in \mathbb{F}_q$ are adjacent if and only if their difference is a cubic residue, *i.e.*, vertex i is adjacent to vertex j if, and only if, $i - j = x^3$ for some $x \in \mathbb{F}_q$. Note that -1 is a cube in $\mathbb{F}_q$ because $q \equiv 1 \pmod 3$ is a prime power, so i is adjacent to j if, and only if, j is adjacent to

i. In [14] it has been proved that $P^3(q)$ has the k-extension property whenever $q \geq k^2 2^{4k-2}$.

The *degree* of vertex v in a graph G is the number $d(v) := |\{\{v,u\} \in E : u \in V_G\}|$ of vertices that are adjacent to v. A graph G is *regular* of degree d if every vertex is adjacent to exactly d other vertices, *i.e.*, $d(v) = d$ for all $v \in V_G$. So, G is regular of degree d if, and only if, each row of its adjacency matrix adds up to d. It is known that the Paley graph $P(q)$ is regular of degree $(q-1)/2$ [15]. Moreover, it has been proved that the cubic Paley graph $P^3(q)$ is regular of degree $(q-1)/3$ [16].

In proving our next result we shall use two lemmas, one is well-known in the literature and other follows from the first. We state them here without proof:

Lemma 1. *Let G be a regular graph of degree d. Then, $d \in \mathrm{sp}(G)$ and for each $\lambda \in \mathrm{sp}(G)$ the absolute value of λ is at most d.*

Lemma 2. *Let G and H be regular graphs of distinct degrees. Then G and H do not have the same spectrum.*

The following result establishes the complete incomparability between cospectrality and elementary equivalence in any finite-variable logic L^k.

Proposition 4. *For each $k \geq 1$, there exists a pair G_k, H_k of non-cospectral graphs such that G_k, H_k are not distinguished by any formula of L^k.*

Proof. For any positive integer r we have that $13^r \equiv 1 \pmod 3$ and $13^r \equiv 1 \pmod 4$. For each $k \geq 1$, let r_k be the smallest integer greater than $2(k\log(4) + \log(k))/\log(13)$, and let $q_k = 13^{r_k}$. Hence $q_k > k^2 2^{4k}$. Now, let $G_k = P(q_k)$ and $H_k = P^3(q_k)$. Then G_k and H_k both satisfy the k-extension property, and so $G_k \equiv^{L^k} H_k$. Since the degree of G_k is $(13^{r_k} - 1)/2$ and the degree of H_k is $(13^{r_k} - 1)/3$, by Lemma 2 we conclude that $\mathrm{sp}(G_k) \neq \mathrm{sp}(H_k)$. $\square$

Therefore, having the same spectrum is a property of graphs that does not follow from any finite collection of extension axioms, or equivalently, from any first-order sentence with asymptotic probability 1. This is because any first-order sentence that has asymptotic probability 1 is a logical consequence of a finite collection of extension axioms [17].

Now, let C^k_m denote the set of first order formulas using at most $k \geq 1$ variables and having quantifier rank at most $m \geq 0$. Cai, Fürer and Immerman in [18, Theorem 5.2] proved that given G and H non-isomorphic graphs, $G \equiv^{C^{k+1}_m} H$ if and only if m iterations of the k-dimensional Weisfeiler-Leman method are not sufficient for distinguishing G and H. Since the first step of the 1-dimensional Weisfeiler-Leman method gives us the degree sequence of both graphs, one iteration is needed for distinguishing graphs with distinct degree sequences. Let $G \cong_d H$ denote that G and H have the same degree sequence. Then, $G \equiv^{C^2_1} H$ if and only if $G \cong_d H$. This notation allows us to establish the following:

Proposition 5. *There are no $k > 1$ and $m > 0$ such that for G and H graphs, if $\mathrm{sp}(G) = \mathrm{sp}(H)$ then $G \equiv^{C^k_m} H$.*

Proof. For a contradiction, suppose there were $k > 1$ and $m > 0$ such that $\mathrm{sp}(G) \neq \mathrm{sp}(H)$ if $G \not\equiv^{C^k_m} H$. Then,

$$\mathrm{sp}(G) = \mathrm{sp}(H) \;\Rightarrow\; G \equiv^{C^k_m} H \;\Rightarrow\; G \equiv^{C^2_1} H \;\Rightarrow\; G \cong_d H.$$

Let $G = C_4 \cup K_1$ and $H = K_{1,4}$. By computing the spectrum of G and H, we have that $\mathrm{sp}(G) = \mathrm{sp}(H) = \{-2, 0, 0, 0, 2\}$. However, the degree sequence of G is $(2, 2, 2, 2, 0)$ and the degree sequence of H is $(4, 1, 1, 1, 1)$. Contradiction. □

In other words, for two graphs, cospectrality does not imply equality of their C^k_m-theories for any $k > 1$ and $m > 0$. Therefore, there is no counting logic that completely captures cospectrality.

4. Isomorphism Approximations

In this section we review some other approximations of graph isomorphism coming from algebra and combinatorics, and relate them to cospectrality. For a certain class of graphs with high combinatorial regularity, we note that cospectrality coincides with C^3-equivalence.

4.1. Cellular Algebras

The automorphism group $\mathrm{Aut}(G)$ of G acts naturally on the set V^k_G of all k-tuples of vertices of G, and the set of orbits of k-tuples under the action of $\mathrm{Aut}(G)$ form a corresponding partition of V^k_G. The *k-dimensional Weisfeiler-Leman algorithm* is a combinatorial method that tries to approximate the partition induced by the orbits of $\mathrm{Aut}(G)$ by labelling the k-tuples of vertices of G. Originally, Weisfeiler and Leman [19] presented their algorithm in terms of algebras of complex matrices. Given two matrices A and B of the same order, their *Schur product* $A \circ B$ is defined by $(A \circ B)_{ij} := A_{ij}B_{ij}$. For a complex matrix A, let A^* denote the adjoint (or conjugate-transpose) of A. A *cellular algebra* W is an algebra (with matrix multiplication) of square complex matrices that contains the identity matrix I, the all-ones matrix J, and is closed under adjoints and Schur multiplication. Thus, every cellular algebra has a unique basis $\{A_1, \ldots, A_m\}$ of binary matrices which is closed under adjoints and such that $\sum_i A_i = J$.

The smallest cellular algebra is the one generated by the span of I and J. The cellular algebra of an n-vertex graph G is the smallest cellular algebra W_G that contains A_G. Two cellular algebras W and W' are isomorphic if there is an algebra isomorphism $h : W \to W'$, such that $h(A \circ B) = h(A) \circ h(B)$, $h(A)^* = h(A^*)$ and $h(J) = J$. Given an isomorphism $h : W \to W'$ of cellular algebras, for all $A \in W$ we have that A and $h(A)$ are cospectral (see Lemma 3.4 in [20]). So the next result is immediate.

Proposition 6. *Two graphs G and H are cospectral if there is an isomorphism of W_G and W_H that maps A_G to A_H.*

In general, the converse of Proposition 6 is not true. That is, there are known pairs of cospectral graphs whose corresponding cellular algebras are non-isomorphic (see, *e.g.* [21]). The elements of the standard basis of a cellular algebra correspond to the "adjacency matrices" of a corresponding coherent configuration. Coherent configurations where introduced by Higman in [22] to study finite permutation groups. Coherent configurations are stable under the 2-dimensional Weisfeiler-Leman algorithm. Hence two graphs G and H are 2-WL equivalent if, and only if, there is an isomorphism of W_G and W_H that maps A_G to A_H:

Proposition 7. *Given graphs G and H with cellular algebras W_G and W_H, $G \equiv^{C^3} H$ if, and only if, there is an isomorphism of W_G and W_H that maps A_G to A_H.*

4.2. Strongly Regular Graphs

A *strongly regular graph* $\mathrm{srg}(n, r, \lambda, \mu)$ is a regular n-vertex graph of degree r such that each pair of adjacent vertices has λ common neighbours, and each pair of nonadjacent vertices has μ common neighbours. The numbers n, r, λ, μ are called the *parameters* of $\mathrm{srg}(n, r, \lambda, \mu)$. It can be shown that the spectrum of a strongly regular graph is determined by its parameters [15]. The complement of a strongly regular graph is strongly regular. Moreover, cospectral strongly regular graphs have cospectral complements. That is, two strongly regular graphs having the same parameters are cospectral. Recall J is the all-ones matrix.

Lemma 3. *If G is a strongly regular graph then $\{I, A_G, (J - I - A_G)\}$ form the basis for its corresponding cellular algebra W_G.*

Proof. By definition, W_G has a unique basis $\mathcal{A}$ of binary matrices closed under adjoints and so that

$$\sum_{A \in \mathcal{A}} A = J.$$

Notice that I, A_G and $J - I - A_G$ are binary matrices such that $I^* = I$, $A_G^* = A_G$ and $(J - I - A_G)^* = J - I - A_G$. Furthermore,

$$I + A_G + (J - I - A_G) = J$$

so $\{I, A_G, (J - I - A_G)\}$ is a basis for W_G indeed. □

There are known pairs of non-isomorphic strongly regular graphs with the same parameters (see, *e.g.* [23]). These graphs are not distinguished by the 2-dimensional Weisfeiler-Leman algorithm since there is an algebra isomorphism that maps the adjacency matrix of one to the adjacency matrix of the other. Thus, for strongly regular graphs the converse of Proposition 6 holds.

Lemma 4. *If G and H are two cospectral strongly regular graphs, then there exists an isomorphism of W_G and W_H that maps A_G to A_H.*

Proof. The cellular algebras W_G and W_H of G and H have standard basis $\{I, A_G, (J - I - A_G)\}$ and $\{I, A_H, (J - I - A_H)\}$, respectively. Since G and H are cospectral, there exist an orthogonal matrix Q such that $QA_GQ^T = A_H$ and $Q(J-I-A_G)Q^T = (J-I-A_H)$. In [20], Friedland has shown that two cellular algebras with standard bases $\{A_1, \ldots, A_m\}$ and $\{B_1, \ldots, B_m\}$ are isomorphic if, and only if, there is an invertible matrix M such that $MA_iM^{-1} = B_i$ for $1 \leq i \leq m$. As every orthogonal matrix is invertible, we can conclude that there exists an isomorphism of W_G and W_H that maps A_G to A_H. □

Proposition 8. *Given two strongly regular graphs G and H, the following statements are equivalent:*

1. $G \equiv^{C^3} H$*;*
2. G *and* H *are cospectral;*
3. *there is an isomorphism of* W_G *and* W_H *that maps* A_G *to* A_H*.*

Proof. Proposition 2 says that for all graphs (1) implies (2). From Proposition 7, we have (1) if, and only if, (3). By Lemma 4, if (2) then (3). □

5. Definability in Fixed Point Logic with Counting

In this section, we consider the definability of cospectrality and the property DS in fixed-point logics with counting. To be precise, we show that cospectrality is definable in *inflationary fixed-point logic with counting* (FPC) and the class of graphs that are DS is definable in *partial fixed-point logic with counting* (PFPC). It follows that both of these are also definable in the infinitary logic with counting, with a bounded number of variables (see [24, Prop. 8.4.18]). Note that it is known that FPC can express any polynomial-time decidable property of *ordered* structures and similarly PFPC can express all polynomial-space decidable properties of ordered structures. It is easy to show that cospectrality is decidable in polynomial time and DS is in PSPACE. For the latter, note that DS can easily be expressed by a Π_2 formula of second-order logic and therefore the problem is in the second-level of the polynomial hierarchy. However, in the absence of a linear order FPC and PFPC are strictly weaker than the complexity classes P and PSPACE respectively. Indeed, there are problems in P that are not even expressible in the infinitary logic with counting. Nonetheless, it is in this context without order that we establish the definability results below.

We begin with a brief definition of the logics in question, to fix the notation we use. For a more detailed definition, we refer the reader to [17, 24].

FPC is an extension of inflationary fixed-point logic with the ability to express the cardinality of definable sets. The logic has two sorts of first-order variables: *element variables*, which range over elements of the structure on which a formula is interpreted in the usual way, and *number variables*, which range over some initial segment of the natural numbers. We usually write element variables with lower-case Latin letters $x, y, \ldots$ and use lower-case Greek letters $\mu, \eta, \ldots$ to denote number variables. In addition, we have relational variables, each of which has an arity m and an associated type from $\{\text{elem}, \text{num}\}^m$. PFPC is similarly obtained by allowing the *partial fixed point* operator in place of the inflationary fixed-point operator.

For a fixed signature σ, the atomic formulas of FPC[σ] of PFPC[σ] are all formulas of the form $\mu = \eta$ or $\mu \leq \eta$, where μ, η are number variables; $s = t$ where s, t are element variables or constant symbols from σ; and $R(t_1, \dots, t_m)$, where R is a relation symbol (*i.e.* either a symbol from σ or a relational variable) of arity m and each t_i is a term of the appropriate type (either elem or num, as determined by the type of R). The set FPC[σ] of FPC *formulas* over σ is built up from the atomic formulas by applying an inflationary fixed-point operator $[\mathbf{ifp}_{R,\vec{x}}\phi](\vec{t})$; forming *counting terms* $\#_x\phi$, where ϕ is a formula and x an element variable; forming formulas of the kind $s = t$ and $s \leq t$ where s, t are number variables or counting terms; as well as the standard first-order operations of negation, conjunction, disjunction, universal and existential quantification. Collectively, we refer to element variables and constant symbols as *element terms*, and to number variables and counting terms as *number terms*. The formulas of PFPC[σ] are defined analogously, but we replace the fixed-point operator rule by the partial fixed-point: $[\mathbf{pfp}_{R,\vec{x}}\phi](\vec{t})$.

For the semantics, number terms take values in $\{0, \dots, n\}$, where n is the size of the structure in which they are interpreted. The semantics of atomic formulas, fixed-points and first-order operations are defined as usual (c.f., *e.g.*, [24] for details), with comparison of number terms $\mu \leq \eta$ interpreted by comparing the corresponding integers in $\{0, \dots, n\}$. Finally, consider a counting term of the form $\#_x\phi$, where ϕ is a formula and x an element variable. Here the intended semantics is that $\#_x\phi$ denotes the number (*i.e.* the element of $\{0, \dots, n\}$) of elements that satisfy the formula ϕ.

Note that, since an inflationary fixed-point is easily expressed as a partial fixed-point, every formula of FPC can also be expressed as a formula of PFPC. In the construction of formulas of these logics below, we freely use arithmetic expressions on number variables as the relations defined by such expressions can easily be defined by formulas of FPC.

5.1. Cospectrality in FPC

In Section 3 we constructed sentences ϕ_k^l of C^3 which are satisfied in a graph G if, and only if, the number of closed walks in G of length l is exactly k. Our first aim is to construct a single formula of FPC that expresses this for all l and k. Ideally, we would have the numbers as parameters to the formula but it should be noted that, while the length l of walks we consider is bounded by the number n of vertices of G, the number of closed walks of length l is not bounded by any polynomial in n. Indeed, it can be as large as n^n. Thus, we cannot represent the value of k by a single number variable, or even a fixed-length tuple of number variables. Instead, we represent k as a binary relation K on the number domain. The order on the number domain induces a lexicographical order on pairs of numbers, which is a way of encoding numbers in the range $0, \dots, n^2$. Let us write $[i, j]$ to denote the number coded by the pair (i, j). Then, a binary relation K can be used to represent a number k up to 2^{n^2} by its binary encoding. To be precise, K contains all pairs (i,j) such that bit position $[i,j]$ in the binary encoding of k is 1. It is easy to define formulas of FPC to express arithmetic operations on numbers represented in this way.

Thus, we aim to construct a single formula $\phi(\lambda, \kappa_1, \kappa_2)$ of FPC, with three free number variables such that $G \models \phi[l,i,j]$ if, and only if, the number of closed walks in G of length l is k and position $[i,j]$ in the binary expansion of k is 1. To do this, we first define a formula $\psi(\lambda, \kappa_1, \kappa_2, x, y)$ with free number variables λ, κ_1 and κ_2 and free element variables x and y that, when interpreted in G defines the set of tuples (l,i,j,v,u) such that if there are exactly k walks of length l starting at v and ending at u, then position $[i,j]$ in the binary expansion of k is 1. This can be defined by taking the inductive definition of ψ_k^l we gave in Section 3 and making the induction part of the formula.

We set out the definition below.

$$\begin{aligned}\psi(\lambda, \kappa_1, \kappa_2, x, y) \quad := \quad & \mathbf{ifp}_{W,\lambda,\kappa_1,\kappa_2,x,y}[(\lambda = 1 \wedge \kappa_1 = 0 \wedge \kappa_2 = 1 \wedge E(x,y)) \vee \\ & \exists \lambda'(\lambda = \lambda' + 1 \wedge \mathrm{sum}(\lambda', \kappa_1, \kappa_2, x, y))]\end{aligned}$$

where W is a relation variable of type $(\mathrm{num}, \mathrm{num}, \mathrm{num}, \mathrm{elem}, \mathrm{elem})$ and the formula sum expresses that there is a 1 in the bit position encoded by (κ_1, κ_2) in the binary expansion of $k = \sum_{z:E(x,z)} k_{\lambda',z,y}$, where $k_{\lambda',z,y}$ denotes the number coded by the binary relation $\{(i,j) : W(\lambda', i, j, z, y)\}$. We will not write out the formula sum in full. Rather we note that it is easy to define inductively the sum of a set of numbers given in binary notation, by defining a sum and carry bit. In our case, the set of numbers is given by a ternary relation of type $(\mathrm{elem}, \mathrm{num}, \mathrm{num})$ where fixing the first component to a particular value z yields a binary relation coding a number. A similar application of induction to sum a set of numbers then allows us to define the formula $\phi(\lambda, \kappa_1, \kappa_2)$ which expresses that the bit position indexed by (κ_1, κ_2) is 1 in the binary expansion of $k = \sum_{x \in V} k_x$ where k_x denotes the number coded by $\{(i,j) : \psi[\lambda, i, j, x, x]\}$.

To define cospectrality in FPC means that we can write a formula cospec in a vocabulary with two binary relations E and E' such that a structure (V, E, E') satisfies this formula if, and only if, the graphs (V, E) and (V, E') are cospectral. Such a formula is now easily derived from ϕ. Let ϕ' be the formula obtained from ϕ by replacing all occurrences of E by E', then we can define:

$$\mathrm{cospec} := \forall \lambda, \kappa_1, \kappa_2 \; \phi \Leftrightarrow \phi'.$$

5.2. DS in PFPC

Now, in order to give a definition in PFPC of the class of graphs that are DS, we need two variations of the formula cospec. This is because we want to universally quantify over graphs E' and say that if E and E' are cospectral, then they are isomorphic. However, we can not universally quantify over sets of edges (*i.e.* binary relations on the element sort), nor can we express isomorphism between E and E' in partial fixed-point logic. Therefore we transfer the graph on E to a number relation R, because here both are possible.

First, let R be a relation symbol of type $(\mathrm{num}, \mathrm{num})$. Note that the number sort has one more element than the element sort, but we can get around this by ignoring the zero. We write $\phi(R)$ for the formula obtained from ϕ by replacing the symbol E with the relation variable R, and suitably replacing number variables with element variables. So, $\phi(R, \lambda, \kappa_1, \kappa_2)$ defines, in the graph defined by the relation R on the number domain, the number of closed walks of length λ. We write cospec_R for the formula

$$\forall \lambda, \kappa_1, \kappa_2\ \phi(R) \Leftrightarrow \phi,$$

which is a formula with a free relational variable R which, when interpreted in a graph G asserts that the graph defined by R is cospectral with G. Similarly, we define the formula with two free second-order variables R and R'

$$\mathrm{cospec}_{R,R'} := \forall \lambda, \kappa_1, \kappa_2\ \phi(R) \Leftrightarrow \phi(R').$$

Clearly, this is true of a pair of relations iff the graphs they define are cospectral.

Furthermore, it is not difficult to define a formula $\mathrm{isom}(R, R')$ of PFPC with two free relation symbols of type $(\mathrm{num}, \mathrm{num})$ that asserts that the two graphs defined by R and R' are isomorphic. Indeed, the number domain is ordered and any property in PSPACE over an ordered domain is definable in PFPC, so such a formula must exist. Given these, the property of a graph being DS is given by the following formula with second-order quantifiers:

$$\forall R(\mathrm{cospec}_R \Rightarrow \forall R'(\mathrm{cospec}_{R,R'} \Rightarrow \mathrm{isom}(R, R'))).$$

To convert this into a formula of PFPC, we note that second-order quantification over the number domain can be expressed in PFPC. That is, if we have a formula $\theta(R)$ of PFPC in which R is a free second-order variable of type $(\mathrm{num}, \mathrm{num})$, then we can define a PFPC formula that is equivalent to $\forall R\, \theta$. We do this by means of an induction that loops through all binary relations on the number domain in lexicographical order and stops if for one of them θ does not hold.

First, define the formula $\mathrm{lex}(\mu, \nu, \mu', \nu')$ to be the following formula which defines the lexicographical ordering of pairs of numbers:

$$\mathrm{lex}(\mu, \nu, \mu', \nu') := (\mu < \mu') \vee (\mu = \mu' \wedge \nu < \nu').$$

We use this to define a formula $\mathrm{next}(R, \mu, \nu)$ which, given a binary relation R of type $(\mathrm{num}, \mathrm{num})$, defines the set of pairs (μ, ν) occurring in the relation that is lexicographically immediately after R.

$$\begin{array}{rcl} \mathrm{next}(R, \mu, \nu) & := & R(\mu, \nu) \wedge \exists \mu' \nu' (\mathrm{lex}(\mu', \nu', \mu, \nu) \wedge \neg R(\mu', \nu')) \vee \\ & & \vee \neg R(\mu, \nu) \wedge \forall \mu' \nu' (\mathrm{lex}(\mu', \nu', \mu, \nu) \Rightarrow R(\mu', \nu')). \end{array}$$

We now use this to simulate, in PFPC, second-order quantification over the number domain. Let $\bar{R}$ be a new relation variable of type $(\mathrm{num}, \mathrm{num}, \mathrm{num})$ and we define the following formula

$$\begin{array}{l} \forall \alpha \forall \beta\, \mathbf{pfp}_{\bar{R}, \mu, \nu, \kappa}[(\forall \mu \nu \bar{R}(\mu, \nu, 0)) \wedge \theta(\bar{R}) \wedge \kappa = 0 \vee \\ \qquad \vee \neg \theta(\bar{R}) \wedge \kappa \neq 0 \vee \\ \qquad \vee \theta(\bar{R}) \wedge \mathrm{next}(\bar{R}, \mu, \nu) \wedge \kappa = 0](\alpha, \beta, 0). \end{array}$$

It can be checked that this formula is equivalent to $\forall R\, \theta$.

5.3. Lower Bounds

We have seen above that cospectrality is definable in FPC and the property DS in PFPC. The use of counting seems essential to these constructions and it is natural to ask whether the properties might be definable in the logics without counting, *i.e.* inflationary fixed-point logic FP and partial fixed-point logic PFP respectively. Or, more plausibly, can we show that this is impossible? Here, we show that it is a consequence of Proposition 4 that cospectrality is not definable in FP.

Proposition 9. *There is no formula of* FP *that defines cospectrality.*

Proof. Suppose, for contradiction, that there was such a formula ϕ. Then, by standard results on FP, there is a k such that if $G \equiv^k H$, then $G \models \phi$ if, and only if, $H \models \phi$. Let G_k and H_k be graphs, as in Proposition 4 that are not cospectral, but $\equiv^k$-equivalent. Now, consider the structures $\bar{GH}_k$ and $\bar{GG}_k$ in the vocabulary with two edge relations E_1 and E_2 defined as follows. Recall that G_k and H_k have the same number of vertices, and let this number be n. Then $\bar{GH}_k$ is defined to be a structure on $2n$ vertices interpreting E_1 as the edges of the graph G_k on the first n vertices and E_2 as the edges of the H_k on the last n vertices. On the other hand, $\bar{GG}_k$ is defined to be a structure on $2n$ vertices interpreting E_1 as the edges of the graph G_k on the first n vertices and E_2 again as the edges of G_k on the last n vertices. It is easily seen that $\bar{GG}_k \models \phi$ while $\bar{GH}_k \not\models \phi$. A simple pebble game argument shows however that $\bar{GH}_k \equiv^k \bar{GG}_k$ yielding the desired contradiction. □

We conjecture that a similar argument would also yield that the property DS is not definable in PFP.

6. Conclusion

Cospectrality is an equivalence relation on graphs with many interesting facets. While not every graph is determined up to isomorphism by its spectrum, it is a long-standing conjecture (see [2]), still open, that *almost all* graphs are DS. That is to say that the proportion of n-vertex graphs that are DS tends to 1 as n grows. We have established a number of results relating graph spectra to definability in logic and it is instructive to put them in the perspective of this open question. It is an easy consequence of the results in [11] that the proportion of graphs that are determined up to isomorphism by their L^k theory tends to 0. On the other hand, it is known that almost all graphs are determined by their C^2 theory (see [25]) and *a fortiori* by their C^3 theory. We have established that cospectrality is incomparable with L^k-equivalence for any k; is incomparable with C^2 equivalence; and is subsumed by C^3 equivalence. Thus, our results are compatible with either answer to the open question of whether almost all graphs are DS. It would be interesting to explore further whether logical definability can cast light on this question.

Now, one could ask what is the complexity of graph isomorphism on graphs that have the same spectrum. Maybe this can be shown to be in the complexity class P. Unfortunately it looks like cospectral graphs tend to be harder to distinguish. An example: all strongly regular graphs with the same parameter set are cospectral. The best algorithm for graph isomorphism of these performs quite badly. From our knowledge, the literature does not contain any specific attempt to graph isomorphism of cospectral graphs apart from the strongly regular ones.

We know no other explicit connection between spectra of other matrices associated with graphs (*e.g.* Laplacian matrices, distance matrices, etc.) and some property of graphs expressible in full first-order logic. We have used the equivalence between cospectrality and satisfying certain structural property, namely having the same total number of closed walks, to capture the spectrum of a graph by writing a logical sentence that counts the number of closed walks.

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