

Descriptive complexity of graph spectra

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Abstract. Two graphs are co-spectral 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 co-spectral 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 co-spectral, 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.

Keywords: descriptive complexity, algebraic graph theory, isomorphism approximations

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. Say that two graphs are co-spectral if they have the same spectrum. Our aim in this paper is to study the relationship of this 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 co-spectrality 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 co-spectral with G . From this, it follows that elementary equivalence in C^3 refines co-spectrality, a result that also follows from [1]. In contrast, we show that co-spectrality 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, co-spectrality exactly co-incides with C^3 -equivalence.

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For definability results, we show that co-spectrality 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 co-spectral 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 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, and establish that co-spectrality on the class of all graphs is refined by C^3 -equivalence. 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 (named after Weisfeiler and Leman) for distinguishing between non-isomorphic graphs, and study the relationship with other algorithms of algebraic and combinatorial nature. Finally, in section 5, we establish some results about the logical definability of co-spectrality and of the property of being a graph determined by its spectrum.

2 Preliminaries

Consider a first-order language $L = \{E\}$, where E is a binary relation symbol interpreted as an irreflexive symmetric binary relation called *adjacency*. Then an L -structure $G = (V_G, E_G)$ is called a *simple undirected graph*. The domain 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 L -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, \dots, v_n is the $n \times n$ matrix A_G with $(A_G)_{ij} = 1$ 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 $A_G P = P A_H$.

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 $\text{sp}(G) := \{\lambda : p_G(\lambda) = 0\}$, where each root of $p_G(\lambda)$ is considered according to its multiplicity. If $\theta \in \text{sp}(G)$ then $\theta I - A_G$ is not invertible, and so there exists a nonzero vector u such that $A_G u = \theta u$. A vector like u is called an *eigenvector*

of G corresponding to θ . The elements in $\text{sp}(G)$ are called the *eigenvalues* of G . Two graphs are called *co-spectral* 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 $\text{tr}(AB) = \text{tr}(BA)$, where $\text{tr}(\cdot)$ is the operation of computing the trace of the matrix inside the parentheses. Therefore, if G and H are two isomorphic graphs then $\text{tr}(A_H) = \text{tr}(P^T A_G P) = \text{tr}(A_G P P^T) = \text{tr}(A_G)$ and so, $\text{tr}(A_G^k) = \text{tr}(A_H^k)$ for any $k \geq 0$.

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 . Assuming that A is an $n \times n$ matrix with (possibly repeated) eigenvalues $\lambda_1, \dots, \lambda_n$, the *elementary symmetric polynomials* e_k in the eigenvalues are the sum of all distinct products of k distinct eigenvalues:

$$\begin{aligned} e_0(\lambda_1, \dots, \lambda_n) &:= 1; & e_1(\lambda_1, \dots, \lambda_n) &:= \sum_{i=1}^n \lambda_i; \\ e_k(\lambda_1, \dots, \lambda_n) &:= \sum_{1 \leq i_1 < \dots < i_k \leq n} \lambda_{i_1} \cdots \lambda_{i_k} && \text{for } 1 \leq k \leq n. \end{aligned}$$

These expressions are the coefficients of the characteristic polynomial of A modulo a 1 or -1 factor. That is,

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

So if we know $s_k(\lambda_1, \dots, \lambda_n) := \sum_{i=1}^n \lambda_i^k$ for $k = 1, \dots, n$, then using *Newton's identities*:

$$e_k(\lambda_1, \dots, \lambda_n) = \frac{1}{k} \sum_{j=1}^k (-1)^{j-1} e_{k-j}(\lambda_1, \dots, \lambda_n) s_j(\lambda_1, \dots, \lambda_n) \quad \text{for } 1 \leq k \leq n,$$

we can obtain all the symmetric polynomials in the eigenvalues, and so we can reconstruct the characteristic polynomial of A .

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

- (i) G and H are co-spectral;
- (ii) G and H have the same characteristic polynomial;
- (iii) $\text{tr}(A_G^k) = \text{tr}(A_H^k)$ for $1 \leq k \leq n$.

3 Spectra and Walks

Given a graph G , 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, \dots, 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, \dots, 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.

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 co-spectral 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 co-spectral non-isomorphic graphs, let $G = C_4 \cup K_1$ and $H = K_{1,4}$, where C_n is the n -vertex cycle, K_n is the complete n -vertex graph, $K_{n,m}$ the complete $(n+m)$ -vertex bipartite graph, and “ \cup ” denotes the disjoint union of two graphs. 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:

$$\psi_0^1(x, y) := \neg E(x, y); \quad \psi_1^1(x, y) := E(x, y);$$

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

For the inductive case, we first introduce some notation. Say that a collection $(i_1, k_1), \dots, (i_r, k_r)$ of pairs of integers, with $i_j \geq 1$ and $k_j \geq 0$ is an *indexed partition* of k if the k_1, \dots, k_r are pairwise distinct and $k = \sum_{j=1}^r i_j k_j$. That is, we partitioned k into $\sum_{j=1}^r i_j$ distinct parts, and there are exactly i_j parts of size k_j where $j = 1, \dots, r$. 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 $l + 1$

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

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

where $d = \sum_{j=1}^r i_j$. 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

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

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, $\text{tr}(A_G^l) = k$. Thus, we have the following proposition.

Proposition 2. *If $G \equiv_C^3 H$ then G and H are co-spectral.*

Proof. Suppose G and H are two non-co-spectral graphs. Then there is some l such that $\text{tr}(A_G^l) \neq \text{tr}(A_H^l)$, i.e. 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 $H \not\models \phi_k^l$. Since ϕ_k^l is a sentence of C^3 , we conclude that $G \not\equiv_C^3 H$. \square

For any graph G and $l \geq 1$, there exists a positive integer k_l such that $\text{tr}(A_G^l) = k_l$. 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

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

of C^3 such that for any graph H , we have $H \models \phi_G$ if, and only if, $\text{sp}(G) = \text{sp}(H)$.

3.2 Graphs Determined by Their Spectra

We say that a graph G is *determined by its spectrum* (for short, DS) when for any graph H , if $\text{sp}(G) = \text{sp}(H)$ 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 co-spectral. That is, if two graphs G and H are C^3 -equivalent then G and H must have the

same spectrum. It thus follows that being identified by C^3 is weaker than being determined by the spectrum, so there are more graphs identified by C^3 than graphs determined by their spectra.

Observation 1 *On the class of all finite graphs, C^3 -equivalence refines co-spectrality.*

In general, determine 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. [22]). 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 [16], from a classical result of Babai, Erdős and Selkow [3], 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 $\text{DS}_n \cap \mathcal{C}_n^2$.

Let T be a tree on n vertices. By a well-known result from Schwenk [21], with probability one there exists another tree T' such that T and T' are co-spectral but not isomorphic. From a result of Immerman and Lander [16] 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, $2K_m$ is DS (see [22, 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 $2K_m$. Hence G_{2m} and $2K_m$ are not distinguishable in C^2 and clearly not isomorphic. This shows that co-spectrality and elementary equivalence with respect to the two-variable counting logic is incomparable.

From a result of Babai and Kučera [4], 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 [18] 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 co-spectrality, 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 co-spectral graphs can be distinguished by a formula using just two variables and no counting quantifiers.

Proposition 3. *There exists a pair of co-spectral graphs that can be distinguished in first-order logic with only two variables.*

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 $C_4 \cup K_1 \models \psi$ and $K_{1,4} \not\models \psi$. Therefore, $C_4 \cup K_1 \not\equiv^2 K_{1,4}$. \square

Next, we show that counting quantifiers are essential to the argument from the previous section in that co-spectrality 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.

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

$$\forall x_1 \dots \forall x_{r+s} \left(\left(\bigwedge_{i \neq j} x_i \neq x_j \right) \rightarrow \exists y \left(\bigwedge_{i \leq r} E(x_i, y) \wedge \bigwedge_{i > r} \neg E(x_i, y) \wedge x_i \neq y \right) \right).$$

A graph G satisfies the *k-extension property* if $G \models \eta_{r,s}$ and $r + s = k$. In [17] Kolaitis and Vardi proved that if the 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 $G \equiv^k H$. Fagin [11] 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 $\text{GF}(q)$, 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 $\text{GF}(q)$ 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 [6] 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 $\text{GF}(q)$, where two vertices $i, j \in \text{GF}(q)$ are adjacent if and only if their difference is a cubic residue, i.e. i is adjacent to j if, and only if, $i - j = x^3$ for some $x \in \text{GF}(q)$. Note that -1 is a cube in $\text{GF}(q)$ 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 [2] 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 can be shown that the Paley graph $P(q)$ is regular of degree $(q-1)/2$ [13]. Moreover, it has been proved that the cubic Paley graph $P^3(q)$ is regular of degree $(q-1)/3$ [10].

Lemma 1. *Let G be a regular graph of degree d . Then $d \in \text{sp}(G)$ and for each $\theta \in \text{sp}(G)$, we have $|\theta| \leq d$. Here $|\cdot|$ is the operation of taking the absolute value.*

Proof. Let us denote by $\mathbf{1}$ the all-ones vector. Then $A_G \mathbf{1} = d\mathbf{1}$. Therefore, $d \in \text{sp}(G)$. Now, let s be such that $|s| > d$. Then, for each row i ,

$$|S_{ii}| > \sum_{j \neq i} |S_{ij}|$$

where $S = sI - A_G$. Therefore, the matrix S is strictly diagonally dominant, and so $\det(sI - A_G) \neq 0$. Hence s is not an eigenvalue of G . \square

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

Proof. Suppose that G is regular of degree s and H is regular of degree t , with $s \neq t$. Then $A_G \mathbf{1} = s\mathbf{1}$ and $A_H \mathbf{1} = t\mathbf{1}$, where $\mathbf{1}$ is the all-ones vector. Therefore, s is the greatest eigenvalue in the spectrum of G and t is the greatest eigenvalue in the spectrum of H . Hence $\text{sp}(G) \neq \text{sp}(H)$. \square

Proposition 4. *For each $k \geq 1$, there exists a pair G_k, H_k of graphs which are not co-spectral, such that G_k and 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 $G_k \equiv^k H_k$. 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 1 we conclude that $\text{sp}(G_k) \neq \text{sp}(H_k)$. \square

So 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.

4 Isomorphism Approximations

4.1 WL Equivalence

The automorphism group $\text{Aut}(G)$ of G acts naturally on the set V_G^k of all k -tuples of vertices of G , and the set of orbits of k -tuples under the action of $\text{Aut}(G)$ form a corresponding partition of V_G^k . The k -dimensional Weisfeiler-Leman algorithm is a combinatorial method that tries to approximate the partition induced by

the orbits of $\text{Aut}(G)$ by labelling the k -tuples of vertices of G . For the sake of completeness, here we give a brief overview of the algorithm.

The 1-dimensional Weisfeiler-Leman algorithm has the following steps: first, label each vertex $v \in V_G$ by its degree $d(v)$. The set $N(v) := \{u : \{v, u\} \in E_G\}$ is called the *neighborhood* of $v \in V_G$ and so, the degree of v is just the number of neighbours it has, i.e. $d(v) = |N(v)|$. In this way we have defined a partition $P_0(G)$ of V_G . The number of labels is equal to the number of different degrees. Hence $P_0(G)$ is the degree sequence of G . Then, relabel each vertex v with the multi-set of labels of its neighbours, so each label $d(v)$ is substituted for $\{d(v), \{d(u) : u \in N(v)\}\}$. Since these are multi-sets they might contain repeated elements. We get then a partition $P_1(G)$ of V_G which is either a refinement of $P_0(G)$ or identical to $P_0(G)$. Inductively, the partition $P_t(G)$ is obtained from the partition $P_{t-1}(G)$, by constructing for each vertex v a new multi-set that includes the labels of its neighbours, as it is done in the previous step. The algorithm halts as soon as the number of labels does not increase anymore. We denote the resulting partition of V_G by P_G^1 .

Now we describe the algorithm for higher dimensions. Recall that we are working in the first-order language of graphs $L = \{E\}$. Now, for each graph G and each k -tuple \mathbf{v} of vertices of G we define the (*atomic type*) of \mathbf{v} in G as the set $\text{tp}_G^k(\mathbf{v})$ of all atomic L -formulas $\phi(\mathbf{x})$ that are true in G when the variables of \mathbf{x} are substituted for vertices of \mathbf{v} . More formally, for $k > 1$ we let

$$\text{tp}_G^k(\mathbf{v}) := \{\phi(\mathbf{x}) : |\mathbf{x}| \leq k, G \models \phi(\mathbf{v})\}$$

where, $|\mathbf{x}|$ denotes the number of entries the tuple \mathbf{x} have, and each $\phi(\mathbf{x})$ is either $x_i = x_j$ or $E(x_i, x_j)$ for $1 \leq i, j \leq k$. Essentially, the formulas of $\text{tp}_G^k(\mathbf{v})$ give us the complete information about the structural relations that hold between the vertices of \mathbf{v} . If $u \in V_G$ and $1 \leq i \leq k$, let \mathbf{v}_i^u denote the result of substituting u in the i -th entry of \mathbf{v} .

For each $k > 1$ the k -dimensional Weisfeiler-Leman algorithm proceeds as follows: first, label the k -tuples of vertices with their types in G , so each k -tuple \mathbf{v} is labeled with $\ell_0(\mathbf{v}) := \text{tp}_G^k(\mathbf{v})$; this induces a partition $P_0^k(G)$ of the k -tuples of vertices of G . Inductively, refine the partition $P_i^k(G)$ of V_G^k by relabelling the k -tuples so that each label $\ell_i(\mathbf{v})$ is substituted for $\ell_{i+1}(\mathbf{v}) := \{\ell_i(\mathbf{v}), \{\ell_i(\mathbf{v}_1^u), \dots, \ell_i(\mathbf{v}_k^u) : u \in V_G\}\}$. The algorithm continues refining the partition of V_G^k until it gets to a step $t \geq 1$, where $P_t^k(G) = P_{t-1}^k(G)$; then it halts. We denote the resulting partition of V_G^k by P_G^k .

Notice that for any fixed $k \geq 1$, the partition P_G^k of k -subsets is obtained after at most $|V_G|^k$ steps. If the partitions P_G^k and P_H^k of graphs G and H are the same multi-set of labels obtained by the k -dimensional Weisfeiler-Leman algorithm, we say that G and H are k -WL equivalent. In [8], Cai, Fürer and Immerman proved that two graphs G and H are C^{k+1} -equivalent if, and only if, G and H are k -WL equivalent.

4.2 Symmetric Powers

The k -th symmetric power $G^{\{k\}}$ of a graph G is a graph where each vertex represents a k -subset of vertices of G , and two k -subsets are adjacent if their symmetric difference is an edge of G . Formally, the vertex set $V_{G^{\{k\}}}$ of $G^{\{k\}}$ is defined to be the set of all subsets of V_G with exactly k elements, and for every pair of k -subsets of vertices $V = \{v_1, \dots, v_k\}$ and $U = \{u_1, \dots, u_k\}$, we have $\{V, U\} \in E_{G^{\{k\}}}$ if, and only if, $(V \setminus U) \cup (U \setminus V) \in E_G$. The symmetric powers are related to a natural generalisation of the concept of a walk in a graph. A k -walk of length l in G is a sequence (V_0, V_1, \dots, V_l) of k -subsets of vertices, such that the symmetric difference of V_{i-1} and V_i is an edge of G for $1 \leq i \leq l$. A k -walk is said to be closed if $V_0 = V_l$. The connection with the symmetric powers is that a k -walk in G corresponds to an ordinary walk in $G^{\{k\}}$. Therefore, two graphs have the same total number of closed k -walks of every length if, and only if, their k -th symmetric powers are co-spectral. For each $k \geq 1$, there exist infinitely many pairs of non-isomorphic graphs G and H such that the k -th symmetric powers $G^{\{k\}}$ and $H^{\{k\}}$ are co-spectral [5].

Alzaga, Iglesias and Pignol [1] have shown that given two graphs G and H , if G and H are $2k$ -WL equivalent, then their k -th symmetric powers $G^{\{k\}}$ and $H^{\{k\}}$ are co-spectral. This two facts combined allow us to deduce the following generalisation of Proposition 2.

Proposition 5. *Given graphs G and H and a positive integer k , if $G \equiv_C^{2k+1} H$ then $G^{\{k\}}$ and $H^{\{k\}}$ are co-spectral.*

4.3 Cellular Algebras

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 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 $\{A_1, \dots, A_m\}$ 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 $h : W \rightarrow W'$, such that $h(A \circ B) = h(A) \circ h(B)$, $h(A)^* = h(A^*)$ and $h(J) = J$. Given an isomorphism $h : W \rightarrow W'$ of cellular algebras, for all $A \in W$ we have that A and $h(A)$ are co-spectral (see Lemma 3.4 in [12]). So the next result is immediate.

Proposition 6. *Two graphs G and H are co-spectral 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 co-spectral graphs whose corresponding cellular algebras are non-isomorphic (see, e.g. [5]). The elements of the standard basis of a cellular algebra correspond to the “adjacency matrices” of a corresponding coherent configuration. Coherent configurations were introduced by Higman in [15] 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 .*

4.4 Strongly Regular Graphs

A *strongly regular graph* $\text{srg}(n, r, \lambda, \mu)$ 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 $\text{srg}(n, r, \lambda, \mu)$. It can be shown that the spectrum of a strongly regular graph is determined by its parameters [13]. The complement of a strongly regular graph is strongly regular. Moreover, co-spectral strongly regular graphs have co-spectral complements. That is, two strongly regular graphs having the same parameters are co-spectral. 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,

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

There are known pairs of non-isomorphic strongly regular graphs with the same parameters (see, e.g. [7]). 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 co-spectral 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 co-spectral, 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 [12], Friedland has shown that two cellular algebras with standard bases $\{A_1, \dots, A_m\}$ and $\{B_1, \dots, B_m\}$ 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 co-spectral;
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 co-spectrality and the property DS in fixed-point logics with counting. To be precise, we show that co-spectrality 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 [9, 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 co-spectrality 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 [9] [20].

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, \dots and use lower-case Greek letters μ, η, \dots 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 τ , the atomic formulas of $\text{FPC}[\tau]$ of $\text{PFPC}[\tau]$ 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 τ ; and $R(t_1, \dots, t_m)$, where R is a relation symbol (i.e. either a symbol from τ 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 $\text{FPC}[\tau]$ of *FPC formulas* over τ is built up from the atomic formulas by applying an inflationary fixed-point operator $[\mathbf{ifp}_{R,x}\phi](\mathbf{t})$; 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 $\text{PFPC}[\tau]$ are defined analogously, but we replace the fixed-point operator rule by the partial fixed-point: $[\mathbf{pfp}_{R,x}\phi](\mathbf{t})$.

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., [9] 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.

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.

$$\psi(\lambda, \kappa_1, \kappa_2, x, y) := \mathbf{ifp}_{W, \lambda, \kappa_1, \kappa_2, x, y} [\lambda = 1 \wedge \kappa_1 = 0 \wedge \kappa_2 = 1 \wedge E(x, y) \vee \lambda = \lambda' + 1 \wedge \text{sum}(\lambda', \kappa_1, \kappa_2, x, y)]$$

where W is a relation variable of type (num, num, num, elem, 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 (elem, num, 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 co-spectrality 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 co-spectral. 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:

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

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 . First, let R be a relation symbol of type (num, num). 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 co-spectral with G . Similarly,

we define the formula with two free second-order variables R and R'

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

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

Furthermore, it is not difficult to define a formula $\text{isom}(R, R')$ of PFPC with two free relation symbols of type (num, 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:

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

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

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

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

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

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 (num, num, num) and we define the following formula

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

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

6 Conclusion

Co-spectrality is an equivalence relation on graphs with many interesting facets. While not every graph is determined upto isomorphism by its spectrum, it is a long-standing conjecture (see [22]), 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 [17] 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 [14]) and *a fortiori* by their C^3 theory. We have established that co-spectrality 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.

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