

Generalizations of k -Weisfeiler-Leman partitions and related graph invariants

Anuj Dawar

Danny Vagnozzi

June 3, 2019

Abstract

The family of Weisfeiler-Leman equivalences on graphs is a widely studied approximation of graph isomorphism with many different characterizations. We give a generalization of these by adding a width parameter r and show that these can be linked to a lifting of the classical Weisfeiler-Leman equivalence defined by Evdokimov and Ponomarenko and a k -boson invariant introduced in the context of quantum random walks. We also prove a characterization in terms of an invertible map game (as introduced by Dawar-Holm) on the complex field, which introduces new parameters that allow us to tease apart some subtle variations of the usual Weisfeiler-Leman equivalences.

1 Introduction

In this paper, we are concerned with *undirected loop-free* graphs. For a graph G , we write $V(G)$ for the set of its vertices and $E(G)$ for the set of its edges. Where the graph is clear from the context, we abbreviate these to just V and E .

The graph isomorphism problem is that of determining whether two graphs G and H are really the same, i.e. there is a bijection $\phi : V(G) \rightarrow V(H)$ such that $\{u, v\} \in E(G)$ if, and only if, $\{\phi(u), \phi(v)\} \in E(H)$. Computationally, the problem is equivalent to the problem of determining the orbits of the automorphism group of a graph G . That is, given a graph G , we wish to partition $V(G)$ into the minimum number of classes so that for any pair of vertices u, v in the same class there is an automorphism of G that takes u to v . More generally, we may wish to partition the k -tuples (for some k) of $V(G)$ into equivalence classes based on the automorphisms. These problems are all equivalent (as long as k is bounded by a constant), in the sense that there are easy polynomial-time reductions between them. None of them is known to be solvable in polynomial-time nor known to be **NP**-complete. Babai has shown [2] that they can be solved in quasi-polynomial time, i.e. by an algorithm running in time $\exp(O(\log n)^c)$ for some constant $c > 1$.

Many algorithmic approaches to the graph isomorphism problem rely on approximating the automorphism partition. That is to say, we aim at partitioning the vertices (or tuples of vertices) of G into a partition that may be coarser than the partition into automorphism classes. A very widely-studied method is given by the k -dimensional Weisfeiler-Leman (WL_k) partitions. These can be defined as giving the coarsest partition of the k -tuples of V into classes P_1, \dots, P_t satisfying a natural *stability condition*. This condition says that two tuples u and v in the same class P_i cannot be distinguished by counting the number of substitutions we can make in them to get a tuple in any class P_j . The WL_k partition of a graph G can be constructed in time $n^{O(k)}$. If there

were a constant k such that the WL_k partition yields the automorphism partition on all graphs, then the graph isomorphism problem would be solvable in polynomial time, but we know this is not the case by a result of Cai et al. [5]. We write $G \equiv_{WL}^k H$ to denote that two graphs are not distinguished by the approximation algorithm for graph isomorphism derived from WL_k . When \vec{u} and \vec{v} are two tuples of vertices in a graph G , of length at most k , we also write $\vec{u} \equiv_{WL}^k \vec{v}$ to mean that they are in the same part of the WL_k partition. It is often more convenient for us to formulate and state results in terms of the equivalence relation on tuples in a graph, which approximates the orbit partition, rather than the equivalence relation between graphs, approximating isomorphism. Nearly everything we say about the equivalence relations also applies to the latter.

The k -dimensional Weisfeiler-Leman method was so named by Babai, who defined this generalization of the classic (or 2-dimensional) algorithm originally given by Boris Weisfeiler and Andrei Leman. In the original definition [18] the stability condition is defined not in the combinatorial terms given by Babai but in terms of *cellular algebras*. These, also called *coherent algebras* [7], are algebras of complex matrices closed under pointwise multiplication. The WL_k partition and the corresponding graph isomorphism approximation are extensively studied because they arise completely naturally in many different contexts and have some strikingly different characterizations. In particular, the partition of V^k into WL_k -equivalence classes is the same as the partition into types in C^{k+1} , the first-order logic with counting quantifiers, restricted to $k + 1$ distinct variables [5], which is also characterized by a $k + 1$ -pebble *bijective game* by Hella [13]. Another closely related characterization, which we do not explore further in this paper relates it to levels of the Sherali-Adams relaxations of the basic integer program for testing isomorphism [1, 16]. In this paper, we do not consider the formulation in terms of logic. Rather, we define the equivalence relation \equiv_C^k , corresponding to equivalence in the logic C^k , through a refinement process with a stability condition that is subtly different to the one that defines the WL_k partition. This difference accounts for the fact that it is \equiv_C^{k+1} that is the same as \equiv_{WL}^k . When we introduce an additional *width* parameter, as explained below, this difference becomes more significant.

In this paper, we add further characterizations to this catalogue. Evdokimov and Ponomarenko [11] describe an alternative way to extend the classical (2-dimensional) Weisfeiler-Leman equivalence to higher dimensions. We call these the k -Evdokimov-Ponomarenko equivalences and we are able to show that it is (upto a multiplicative factor of 3 in the dimension) the same as the family of k -dimensional Weisfeiler-Leman equivalences. We also show a connection with a graph invariant defined in terms of k -particle quantum walks introduced in [17].

Dawar and Holm [8] define yet another family of approximations of the orbit partition of a graph, based on a two-player game they call the *invertible map game*. Essentially, this yields a partition P_1, \dots, P_t of the k -tuples of V satisfying a stability condition where every k -tuple \vec{u} induces a partition of V^2 (or, more generally, V^{2m} for some $2m \leq k$ if we add a width parameter $r = 2m$) and for any pair of k -tuples \vec{u} and \vec{v} in the same part P_i , there is an invertible linear map witnessing the equivalence of the partitions induced by u and v . The precise definition is given below in Section 7. This family of approximations is shown to be strictly stronger (i.e. producing a finer approximation) than the Weisfeiler-Leman equivalences if we take these maps to be over a field \mathbb{F} of characteristic p . If we consider only invertible maps over the complex field (or, indeed, any field of characteristic 0), we can show that the family of equivalences $\equiv_{IM}^{k,r}$ interleaves with the family of equivalences \equiv_{WL}^k . We give a proof of this result.

It is an open question whether increasing the value of the width r leads to finer equivalences. Indeed, this question can be reflected back to the equivalences \equiv_{WL}^k where it seems width has

not previously been considered as a parameter. This is partly because (as we see below), in the context of the equivalence \equiv_C^k , width $r > 1$ adds nothing, and it has been implicitly assumed that the same holds for \equiv_{WL}^k . Though the partition into \equiv_C^{k+1} -equivalence classes and \equiv_{WL}^k -equivalence classes leads to the same end result, the refinement process that gets us there is distinct. We can understand the first as a *position-wise* refinement process and the latter as a *tuple-wise* refinement process. This shows that the width parameter is potentially more significant in the case of \equiv_{WL}^k . In the same way, in the context of the invertible map equivalences \equiv_{IM}^k , we can also consider the variations obtained by position-wise and tuple-wise refinement. We show that the two still lead to interleaved partitions (with a small additive term in k).

It is convenient to formulate the comparisons of these various families of algorithms in terms of *Schurian polynomial approximation schemes*, a formalism introduced by Evdokimov and Ponomarenko [11]. We give the definition below in Section 4.

2 Preliminaries

We introduce some notation and definitions that we use in the rest of the paper.

By $[k]$ we mean the set of integers from 1 to k . We use vector notation \vec{v} for tuples. If \vec{v} is a k -tuple, then v_i (for $i \in [k]$) denotes its i^{th} entry. We define $[k]^{(r)} := \{\tau \in [k]^r \mid \tau_i = \tau_j \implies i = j\}$. That is, it is the collection of r -tuples from $[k]$ in which all entries are distinct.

Let $\vec{\tau} \in [k]^{(r)}$ for $r < k$. Let $\vec{v} \in V^k$ and $\vec{x} \in V^r$. We denote by $\vec{v}\langle\vec{\tau}, \vec{x}\rangle \in V^k$ the tuple with i th entry

$$\vec{v}\langle\vec{\tau}, \vec{x}\rangle = \begin{cases} x_{\tau_j} & \text{if } i = \tau_j \text{ for some } j \in [r] \\ v_i & \text{otherwise.} \end{cases} \quad (1)$$

In other words $\vec{v}\langle\vec{\tau}, \vec{x}\rangle$ is the tuple obtained by substituting \vec{x} into \vec{v} in the positions specified by $\vec{\tau}$. If $\vec{v} \in V^k$ and $\vec{\tau}$ and r are as above. We let $\vec{v}[\vec{\tau}] \in V^{k-r}$ be the $(k-r)$ -tuple obtained by removing the v_{τ_i} entries from \vec{v} for all $i \in [r]$.

We use the language of partitions and equivalence relations interchangeably. We also use *labelled* or *coloured* partitions. For a set S , a colouring of S with a set of colours \mathcal{C} is a function $f : S \rightarrow \mathcal{C}$. It induces the equivalence relation \sim where $x \sim y$ iff $f(x) = f(y)$. We call this the *coloured partition* where each part $[x]$ (i.e. the equivalence class containing x) receives the colour $f(x)$.

As remarked above, for a graph G , $V(G)$ and $E(G)$ denote the vertex set and edge set respectively. Where there is no ambiguity, we may simply write V and E . For a k -tuple \vec{v} of vertices from V , the *atomic type* of \vec{v} is the *ordered* graph on the set $[k]$ where i and j are adjacent if, and only if, v_i and v_j are adjacent in G . Two tuples have the same atomic type if the order-preserving map between their atomic types is a graph isomorphism. This induces a coloured partition of V^k where \vec{v} is coloured by its atomic type.

For a finite set S , with a total order on its elements, we denote by $(v_i)_{i \in S}$ (with $v_i \in V$) the vector in $V^{|S|}$ whose i th entry is labelled by the i th element of S in its increasing order.

3 Algebraic aspects

This section is by no means a complete review of our current knowledge on coherent configurations and algebras. For a deeper understanding, see [7].

3.1 Coherent configurations & algebras

Let $\mathcal{R} = \{R_1, \dots, R_m\}$ be a collection of binary relations on a finite set V .

Definition 3.1 (Coherent configuration). *We say that \mathcal{R} forms a coherent configuration on V if:*

1. \mathcal{R} is a partition of V^2 .
2. If $R \in \mathcal{R}$, then $R^t \in \mathcal{R}$, where $R^t = \{(v, u) \in V^2 \mid (u, v) \in R\}$.
3. There is a set $\mathcal{I} \subset \mathcal{R}$ which forms a partition of the diagonal of V , that is, $\bigcup \mathcal{I} = \{(v, v) \mid v \in V\}$.
4. For any $i, j, k \in [m]$, there is a constant p_{ij}^k such that

$$p_{ij}^k = |\{x \in V \mid (x, v) \in R_i\} \cap \{x \in V \mid (u, x) \in R_j\}| \quad (2)$$

for all $(u, v) \in R_k$. In other words, this number is independent of the choice of $(u, v) \in R_k$.

The integer constants p_{ij}^k are called *intersection constants*. A set $S \subseteq V$ is called a *cell* of \mathcal{R} if $S = \{v \mid (v, v) \in R\}$ for some $R \in \mathcal{I}$.

Let $\mathcal{A}_{\mathcal{R}} = \{A(R_i) \mid R_i \in \mathcal{R}\}$, where $A(R_i)$ is the matrix with rows and columns indexed by V whose (u, v) entry is 1 if $(u, v) \in R_i$, and 0 elsewhere. Then the following four conditions amount to an alternative formulation of the requirement that \mathcal{R} forms a coherent configuration:

1. $\sum_{1 \leq i \leq m} A(R_i) = J$ where J is the matrix with each entry equal to 1.
2. For some $\mathcal{I} \subset \mathcal{R}$, $\sum_{R \in \mathcal{I}} A_R = \mathbb{I}$.
3. For each i , there is some j such that $A(R_i)^t = A(R_j)$.
4. There are constants p_{ij}^k such that $A(R_i)A(R_j) = \sum_{1 \leq k \leq m} p_{ij}^k A(R_k)$.

It follows from (2) and (4), that the span of $\mathcal{A}_{\mathcal{R}}$ over \mathbb{C} forms a unital matrix algebra which is semi-simple by (3) (see [6, Chapter 3] for more technical details). Furthermore, $\mathcal{A}_{\mathcal{R}}$ is the unique basis of this algebra satisfying the four conditions above. Finally, this algebra is a *coherent algebra* in the sense of the definition below.

Definition 3.2 (Coherent algebra). *A matrix algebra over \mathbb{C} is said to be a coherent algebra if it is closed under Schur-Hadamard (component-wise) multiplication and it contains the identity matrix \mathbb{I} and the all 1s matrix J .*

Indeed, any coherent algebra arises from a coherent configuration in this way.

In [7] it is shown how one may compute the irreducible modules of a coherent algebra solely from the intersection constants. The most useful application of this idea is that of showing non-existence of coherent algebras with certain intersection constants.

3.2 Morphisms

Coherent configurations arise naturally when studying permutation groups. In fact, if G is a group acting on a set V , then the orbits of the canonical action of G on V^2 form a coherent configuration. The corresponding algebra is the set of complex matrices commuting with the matrices of the permutation representation of G on V , that is:

$$Z(G, V) = \{A \in \text{Mat}_V(\mathbb{C}) \mid A\pi(g) = \pi(g)A \ \forall g \in G\} \quad (3)$$

where $\pi(g)$ is the permutation matrix corresponding to g , i.e.:

$$\pi(g)(u, v) = \begin{cases} 1 & \text{if } g \cdot v = u \\ 0 & \text{elsewhere} \end{cases} \quad (4)$$

Definition 3.3 (Isomorphism of coherent configurations). *Let $\mathcal{R} = \{R_1, \dots, R_m\}$ and $\mathcal{S} = \{S_1, \dots, S_m\}$ be coherent configurations on V and W respectively. We say that a bijection $\phi : V \rightarrow W$ is an isomorphism if for every $i \in [m]$ there is a $j \in [m]$ such that $(x, y) \in R_i \iff (\phi(x), \phi(y)) \in S_j$.*

Let p_{ij}^k and q_{ij}^k be the intersection constants of \mathcal{R} and \mathcal{S} respectively. Clearly, ϕ induces a map $\psi : [m] \rightarrow [m]$ such that $p_{ij}^k = q_{\psi(i)\psi(j)}^{\psi(k)}$. However, not every map that preserves the intersection constants arises from a bijection between V and W . This motivates the following definition.

Definition 3.4 (Weak isomorphism). *Let $\mathcal{R} = \{R_1, \dots, R_m\}$ and $\mathcal{S} = \{S_1, \dots, S_m\}$ be coherent configurations on V and W respectively. Let $\Phi : \mathcal{R} \rightarrow \mathcal{S}$ be a bijection and $\phi : [m] \rightarrow [m]$ be the induced map in the sense: $\Phi(R_i) = S_j \iff \phi(i) = j$. Then Φ is a weak isomorphism if $p_{ij}^k = q_{\phi(i)\phi(j)}^{\phi(k)}$ for all $i, j, k \in [m]$, where p_{ij}^k and q_{ij}^k are the intersection constants of \mathcal{R} and \mathcal{S} respectively.*

It is easy to see how the above definitions are translated in an algebraic setting. However, it turns out that the notion of weak isomorphism is equivalent to the natural notion of isomorphism for coherent algebras. For consistency, we also call this weak isomorphism.

Definition 3.5. *Let W_1 and W_2 be coherent algebras over V_1 and V_2 respectively, with $|V_1| = |V_2|$. A bijection $\iota : W_1 \rightarrow W_2$ is a weak isomorphism if it is an algebra isomorphism and if $\iota(A \cdot B) = \iota(A) \cdot \iota(B)$ for all $A \in W_1, B \in W_2$, where \cdot is the Schur-Hadamard product.*

The fact that ι is an algebra isomorphism ensures that the product of any two elements is mapped onto the product of their respective images and thus, the intersection constants are preserved. Also, preserving the Schur-Hadamard product of two elements ensures that ι maps elements of the standard basis of W_1 to elements of the standard basis of W_2 . Thus, it can be shown that two coherent configurations are weakly isomorphic if, and only if, the coherent algebras they generate are weakly isomorphic.

The following result [12] makes the idea of isomorphism more concrete in the algebraic setting, by establishing that any such isomorphism is actually witnessed by a unitary matrix.

Lemma 3.6 (Friedland, 1989). *Let W_1 and W_2 be coherent algebras on V and W with standard bases $\mathcal{A}_{\mathcal{R}} = \{A(R_1), \dots, A(R_m)\}$ and $\mathcal{A}_{\mathcal{S}} = \{A(S_1), \dots, A(S_m)\}$ respectively. If there is a weak isomorphism $\iota : W_1 \rightarrow W_2$ then there is a unitary matrix U such that, for all i , $UA(R_i)U^\dagger = A(S_j)$, where $\iota(A(R_i)) = A(S_j)$.*

In particular, we may take U to be a permutation matrix whenever ι is induced by a bijection between V and W . Moreover, from this result we can deduce another property.

Lemma 3.7. *Let $\mathcal{R} = \{R_1, \dots, R_m\}$ and $\mathcal{S} = \{S_1, \dots, S_m\}$ be coherent configurations and $\Phi : \mathcal{R} \rightarrow \mathcal{S}$ a weak isomorphism inducing a map $\phi : [m] \rightarrow [m]$. Then $|R_i| = |S_{\phi(i)}|$ for all $i \in [m]$.*

Proof. It is sufficient to show that if S is some invertible matrix such that $SJ = JS$, and $SBS^{-1} = A$ for some boolean matrices A and B , then A and B have the same number of non-zero entries. Indeed, $JB = \beta J$ where β is the number of non-zero entries in B . Also, $\alpha J = JAJ = JSBS^{-1}J = SJBJS^{-1} = \beta J$, from which the desired result follows. \square

We now consider isomorphisms from a coherent configuration to itself.

Definition 3.8 (Weak automorphism). *Let $\mathcal{R} = \{R_1, \dots, R_m\}$ be a coherent configuration on V and $\Phi : \mathcal{R} \rightarrow \mathcal{R}$ a bijection which induces $\phi : [m] \rightarrow [m]$ in the sense explained above. Then Φ is a weak isomorphism if $p_{ij}^k = p_{\phi(i)\phi(j)}^{\phi(k)}$ for all $i, j, k \in [m]$, where p_{ij}^k are the intersection constants of \mathcal{R} .*

Thus, a weak automorphism of \mathcal{R} is just an isomorphism from \mathcal{R} to itself. Our definition of automorphism, however, is different.

Definition 3.9 (Automorphism). *Let $\mathcal{R} = \{R_1, \dots, R_m\}$ be a coherent configuration on V and $\phi : V \rightarrow V$ a bijection. We say that ϕ is an automorphism of \mathcal{R} if $(u, v) \in R_i \iff (\phi(u), \phi(v)) \in R_i$ for all $i \in [m]$.*

Note that not every isomorphism of \mathcal{R} to itself is an automorphism. The conditions imposed on an automorphism are stronger, in that we do not allow any permutation of the index set $[m]$. This will be useful later. We denote by $\text{Aut}(\mathcal{R})$ the set of automorphisms of a coherent configuration \mathcal{R} , and we adopt a similar notation for the algebraic analogue, where, if W is a coherent configuration, then

$$\text{Aut}(W) = \{g \in \text{Sym}(V) \mid A\pi(g) = \pi(g)A \ \forall A \in W\}, \quad (5)$$

where $\pi(g)$ is the permutation matrix corresponding to g . To conclude this subsection we would like to note the two following facts:

1. Not all coherent configurations can be described in terms of group actions.
2. Whilst all automorphisms are also weak automorphisms, the converse does not hold.

4 Schurian polynomial approximation schemes

We now make explicit the connection between coherent configurations and approximations of the graph isomorphism problem. As noted earlier, we approach the latter through the equivalent problem of approximating the partition of a graph into the orbits of its automorphism group.

First, we note that the set of partitions of V^2 form a poset under the relation \preceq whereby two partitions \mathcal{P}_1 and \mathcal{P}_2 satisfy $\mathcal{P}_1 \preceq \mathcal{P}_2$ if, and only if, \vec{u} is in the same class as \vec{v} in \mathcal{P}_2 implies that \vec{u} is in the same class as \vec{v} in \mathcal{P}_1 . More colloquially, one would say that \mathcal{P}_2 is a refinement of \mathcal{P}_1 . It is easy to see that any two partitions \mathcal{P}_1 and \mathcal{P}_2 have unique *greatest lower bounds* and *least upper bounds* with respect to this ordering. That is, the partitions of V^2 form a *lattice*. If we restrict the

relation \preceq to the set of coherent configurations on V , then these still form a lattice, though the least upper bounds and greatest lower bounds may be different from those of general partitions. For a proof of this claim, see [7]. Thus, we can define a similar relation on the set of coherent algebras on V , where we analogously use the symbol \leq , which is the same as the one used to indicate algebraic containment for obvious reasons. Thus, two coherent algebras W_1 and W_2 with respective coherent configurations \mathcal{R}_1 and \mathcal{R}_2 satisfy $W_1 \leq W_2$ if and only if $\mathcal{R}_1 \preceq \mathcal{R}_2$.

The k -dimensional Weisfeiler-Leman algorithm can be seen as computing a coherent configuration. The higher the value of k , the finer the partition obtained, with the partition into automorphism orbits being the limit. This general model of a family of algorithms was formalized into the notion of a *Schurian polynomial approximation scheme*, introduced by Evdokimov et. al. in [11]. This provides a formal setting for us to compare different variations that compute different families of approximations of isomorphism.

Definition 4.1 (Schurian polynomial approximation). *Let $X = \{X_1, \dots, X_k, \dots\}$ be a set of functions mapping coherent configurations on V to coherent configurations on V . We say that X forms a Schurian polynomial approximation scheme (SPAS) if for any coherent configuration \mathcal{R} :*

1. $X_1(\mathcal{R}) = \mathcal{R} \preceq \dots \preceq X_n(\mathcal{R}) = X_{n+1}(\mathcal{R}) = \dots = \text{Sch}(\mathcal{R})$ where $n = |V|$ and $\text{Sch}(\mathcal{R})$ is the coherent configuration arising from the action of $\text{Aut}(\mathcal{R})$ on V .
2. $X_k(X_{k'}(\mathcal{R})) = X_{k'}(\mathcal{R})$ for all $k \leq k'$.
3. $X_k(\mathcal{R})$ can be constructed in $n^{O(k)}$ computational steps.

We call $\text{Sch}(\mathcal{R})$ the *Schurian* of \mathcal{R} . Similarly for a coherent algebra W , $Z(\text{Aut}(W), V)$ is the *Schurian* of W and we denote it by $\text{Sch}(W)$.

For the purpose of studying graphs, we mainly concentrate on a very particular coherent configuration. For a partition R_1, \dots, R_r of V^2 , we write $[R_1, \dots, R_r]$ to denote the coarsest coherent configuration that is a refinement of the partition. When $E \subseteq V^2$, we write $[E]$ as a shorthand for $[E, V^2 \setminus E]$. Analogously, when A_1, \dots, A_r are a collection of 0-1 matrices with $\sum_{1 \leq i \leq r} A_i = J$, we write $[A_1, \dots, A_r]$ for the coherent algebra generated by the corresponding partition.

Lemma 4.2. *Let G be a graph with edge set E and set $\mathcal{R}_G = [E]$.*

$$\text{Aut}(\mathcal{R}_G) = \text{Aut}(G).$$

Proof. Clearly, $\text{Aut}(\mathcal{R}_G) \leq \text{Aut}(G)$, as any automorphism of \mathcal{R}_G must be a permutation preserving the relation E , and is thus in $\text{Aut}(G)$. Let \mathcal{S} be the coherent configuration arising from the action of $\text{Aut}(G)$ on V . Then $\text{Aut}(G) \leq \text{Aut}(\mathcal{S})$. However, \mathcal{S} contains a refinement of E , so it must be a *finer* partition than \mathcal{R}_G , by the definition of the latter. Hence, $\text{Aut}(\mathcal{R})$ cannot be a strict subgroup of $\text{Aut}(\mathcal{S})$ for otherwise, \mathcal{S} would be a coarser partition than \mathcal{R} . As such, we have that $\text{Aut}(\mathcal{R}_G) \leq \text{Aut}(G) \leq \text{Aut}(\mathcal{S}) \leq \text{Aut}(\mathcal{R})$, and the result follows. \square

Corollary 4.3.

$$\text{Aut}(\text{Sch}(\mathcal{R}_G)) = \text{Aut}(G).$$

Proof. For any coherent configuration \mathcal{R} , we have that $\mathcal{R} \preceq \text{Sch}(\mathcal{R})$. From this, we can deduce that $\text{Aut}(\mathcal{R}) \leq \text{Aut}(\text{Sch}(\mathcal{R})) \leq \text{Aut}(\mathcal{R})$, where the first containment follows from the definition of $\text{Sch}(\mathcal{R})$. By taking $\mathcal{R} = \mathcal{R}_G$ the result follows. \square

Thus, if we could find $\text{Sch}(\mathcal{R}_G)$ in polynomial time, then we can obtain the partition into automorphism orbits in polynomial time. In particular, if we had a Schurian polynomial approximation scheme $X = \{X_1, \dots, X_k, \dots\}$ and a fixed k such that $X_k(\mathcal{R}_G) = \text{Sch}(\mathcal{R}_G)$, then it follows that the partition into automorphism orbits can be computed in time $n^{O(k)}$, and the graph isomorphism problem is in polynomial time.

It should be remarked that the reduction from computing the automorphism orbits to the graph isomorphism problem proceeds by considering disjoint unions of graphs. That is, we can determine whether two graphs G and H are isomorphic by computing the orbit partition on their disjoint union $G \oplus H$. In particular, if \mathcal{C} is a class of graphs closed under disjoint unions, and $X = \{X_1, \dots, X_k, \dots\}$ is a Schurian polynomial approximation scheme for which $X_k(\mathcal{R}_G) = \text{Sch}(\mathcal{R}_G)$ for all graphs in \mathcal{C} , then graph isomorphism is polynomial-time decidable on \mathcal{C} . This implication does not hold when \mathcal{C} is not closed under disjoint unions.

The formalism of SPAS allows us to compare different families of algorithms for graph isomorphism. The comparison between families is defined next.

Definition 4.4 (Simulation and equivalence of SPAS). *Let $X = \{X_i\}_{i \in \mathbb{N}}$ and $Y = \{Y_i\}_{i \in \mathbb{N}}$ be SPAS. We say that X simulates Y if for any coherent configuration \mathcal{R} and any $k \in \mathbb{N}$, there is a map $h : \mathbb{N} \rightarrow \mathbb{N}$ such that $Y_k(\mathcal{R}) \preceq X_{h(k)}(\mathcal{R})$. We say that X and Y are equivalent if they simulate each other. If X simulates Y but Y does not simulate X , we say that X improves Y .*

We now see how this provides a framework for comparing families of algorithms. The families we are interested in all provide, for each k , a refinement process that takes a partition of V^k and refines it. In other words, it defines a monotone map on the lattice of partitions of V^k . This yields a limit partition, where we start with the partition of V^k into atomic types and repeatedly refine until we reach a fixed-point of this monotone map. Let $(M_k)_{k \in \mathbb{N}}$ be a family of such monotone maps. We say that a partition P of V^k is M_k -stable if $M_k(P) = P$.

To fit this family of algorithms into the formalism of SPAS defined above, we introduce some more notation. For a tuple $\vec{v} \in V^j$, for $j < k$, define the k -extension of \vec{v} to be the k -tuple obtained from \vec{v} by repeating the last entry $k - j$ times. Given a partition \mathcal{P} of V^k (for $k \geq 2$), define its j -projection, for $j < k$ to be the partition of V^j such that \vec{u} and \vec{v} are in the same class if, and only if, their k -extensions are in the same class of \mathcal{P} . We write $\overline{\mathcal{P}}$ to denote the 2-projection of \mathcal{P} . Likewise, for $j < k$ we define the j -projection of a tuple $\vec{v} \in V^k$ to be the tuple $w \in V^j$ such that $w_i = v_i$ for $i \in [j]$.

Conversely, given a partition \mathcal{Q} of V^2 , we define its k -lift to be the partition $\eta^k(\mathcal{Q})$ of V^k such that two tuples \vec{u} and \vec{v} are equivalent if, and only if, for all $i, j \in [k]$, (u_i, u_j) is \mathcal{Q} -equivalent to (v_i, v_j) .

With these definitions, we can see the procedure M_k as defining a map \overline{M}_k on coherent configurations on V , where $\overline{M}_k(\mathcal{R})$ is defined to be $\overline{M}_k([\eta^k(\mathcal{R})])$, i.e. the coherent configuration generated by the 2-projection of M_k applied to the k -lift of \mathcal{R} . This will, in general be a Schurian polynomial approximation scheme.

To apply such a scheme to the graph isomorphism problem means that we try and approximate the orbit partition on graph by starting with a partition of V^k into atomic types and repeatedly M_k until we get a partition that is M_k -stable. Let ι^k be the colouring of V^k by means of atomic types. So, $\iota^k(\vec{v}) = \iota^k(\vec{w})$ if the map $v_i \rightarrow w_i$ is an isomorphism between the subgraphs of $G = (V, E)$ induced by \vec{v} and \vec{w} respectively. We write \equiv_M^k for the equivalence relation on V^k induced by the coarsest M_k -stable partition that is no coarser than ι^k . More generally, for $j \in [k]$ and two tuples

$\vec{u}, \vec{v} \in V^j$, we write $\vec{u} \equiv_M^j \vec{v}$ if their k -extensions are \equiv_M^k -equivalent. Similarly, if $\vec{u}, \vec{v} \in V^k$, we write $\vec{u} \equiv_M^j \vec{v}$ if their j -projections are \equiv_M^j equivalent.

5 Weisfeiler-Leman refinements

In this section we review some algebraic and combinatorial properties of the k -dimensional Weisfeiler-Leman equivalences. These are known to be the same as equivalence in the $k + 1$ -variable logic with counting (see [5]). Here, we avoid the use of logic, and define the latter in terms of a different combinatorial refinement. This shows a subtle difference between the two refinement algorithms when we introduce a new “width” parameter. In the first part of the section, we review known results, which allows us to establish a common notation for the different refinement procedures.

5.1 The algorithm

The k -Weisfeiler-Leman algorithm in its most general form consists in the following iterative procedure:

- INPUT: a coloured partition f_0 of V^k .
 - OUTPUT: a coloured partition f of V^k .
1. Set $i = 0$.
 2. For all $\vec{v} \in V^k$ and $x \in V$ define the vector

$$S_i(\vec{v}, x) = (f_i(\vec{v}\langle j, x \rangle))_{j \in [k]} \quad (6)$$

Define also the formal sum

$$\sum_{x \in V} S_i(\vec{v}, x) \quad (7)$$

and set

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), \sum_{x \in V} S_i(\vec{v}, x)). \quad (8)$$

3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ then output $f = f_i(\vec{v})$. Otherwise, repeat from step (2).

We denote the output partition induced by f by $\text{WL}_k(f_0)$. More generally, where it does not cause confusion, we also write f for the partition (i.e. ignoring the labels) induced by f . Note that $\text{WL}_k(f_0)$ is indeed coarsest partition of V^k refining f_0 and satisfying $f = \text{WL}_k(f)$. In particular, if $k = 2$ and f_0 is the partition of V^2 into edges, non-edges and the diagonal of some graph G , then $\text{WL}_2(f_0)$ is indeed \mathcal{R}_G . We say that a partition f of V^k is *k-Weisfeiler-Leman stable* if $\text{WL}_k(f) = f$.

By the discussion at the end of the last section, we can see $\overline{\text{WL}}_k$ as a map on coherent configurations. Indeed, we can now establish the main conclusion.

Lemma 5.1. *The family of maps $\{\overline{\text{WL}}_k\}_{k \in \mathbb{N}}$ is a Schurian polynomial approximation scheme.*

The k -dimensional Weisfeiler-Leman algorithm is often described as starting with the partition of V^k into atomic types. The partition this yields under WL_k refinement is the same as if we begin with the smallest coherent configuration refining $[E]$.

Lemma 5.2. *Let \mathcal{R} be the coarsest coherent configuration refining the partition of V^2 into edges, non-edges and the diagonal of V . Then the partitions $\text{WL}_k(\iota^k)$ and $\text{WL}_k(\eta^k(\mathcal{R}))$ are identical.*

We prove this in the next subsection, after introducing the C_k -colouring scheme.

5.2 C_k colouring scheme

The C_k -colouring scheme provides another family $C = \{C_k\}_{k \in \mathbb{N}}$ of approximations of graph isomorphism which turns out to be equivalent to WL_k . We define it by a refinement procedure, as we did for WL_k

- INPUT: a coloured partition f_0 of V^k .
- OUTPUT: a coloured partition f of V^k .
 1. Set $i = 0$.
 2. For each $j \in [k]$ and $\vec{v} \in V^k$ define the formal sum

$$S_j^i(\vec{v}) = \sum_{x \in V} f(\vec{v}\langle j, x \rangle). \quad (9)$$

3. Set

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), (S_j^i(\vec{v}))_{j \in [k]}). \quad (10)$$

4. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^k$ then output $f = f_i$. Else, return to step (2).

We denote the output of this refinement by $C_k(f_0)$ and define C_k stability analogously to what we did for WL_k above. Again, it is clear that this algorithm outputs the coarsest C_k stable partition of V^k refining f_0 , and that when taking $f_0 = \iota^k$ for some graph G , we interpret $C_k(\iota^k)$ to be an approximation of the orbits of the action of the automorphism group of G on V^k .

It is worth highlighting the difference between this refinement procedure and that for WL_k . In defining the colour $f_{i+1}(\vec{v})$ of a tuple, we take into account the colour $f_i(\vec{v})$ at the previous stage and, for each j , the multiset of colours obtained by substituting vertices at the j th position in \vec{v} . In contrast, in the WL_k refinement, $f_{i+1}(\vec{v})$ depends on the multiset of k -tuples of colours, one for each vertex x , obtained by substituting x in the k possible positions in \vec{v} . Thus, in a sense, the WL_k refinement process is carrying more information. Indeed, for any partition f , we have $C_k(f) \preceq \text{WL}_k(f)$. One immediate consequence is that any partition that is WL_k stable is also C_k stable.

Another way we can strengthen the C_k refinement process, that seems orthogonal to taking tuples of colours, is to consider the substitution of r -tuples, for some $r < k$ rather than of a single vertex. As we see below, this does not lead to a strengthening, but it does help us in proving Lemma 5.2 above.

We now define the $C_{k,r}$ refinement procedure as follows:

- INPUT: a coloured partition f_0 of V^k .
- OUTPUT: a coloured partition f of V^k .
 1. Set $i = 0$.

2. For each $\tau \in [k]^{(r)}$ and $\vec{v} \in V^k$ define the formal sum

$$S_\tau^i(\vec{v}) = \sum_{\vec{x} \in V^r} f(\vec{v}\langle\tau, \vec{x}\rangle). \quad (11)$$

3. Set

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), (S_\tau^i(\vec{v}))_{\tau \in [k]^{(r)}}). \quad (12)$$

4. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^k$ then output $f = f_i$. Else, return to step (2).

As before, we denote the output f by $C_{k,r}(f_0)$, and we define $C_{k,r}$ stability as one would expect. Note that $C_{k,1}$ is just C_k . The following is a very useful combinatorial property.

Lemma 5.3. *Any partition f of V^k that is C_k stable is also $C_{k,r}$ stable for all $r < k$.*

Proof. We show this by induction. The case $r = 1$ is true by definition. Suppose that for $r = m$ our desired statement holds true. Let $\vec{\tau} \in [k]^m$ and $\tau_n \in [k]$ be such that it is not an entry of τ . Label equivalence classes of f by f_1, \dots, f_c , and for $i, j \in [c]$ define

$$\lambda_{ij} = |\{x \in V \mid \vec{v}\langle\tau_n, x\rangle \in f_j\}| \quad (13)$$

for some $\vec{v} \in f_i$, and similarly let

$$\mu_{ij} = |\{\vec{x} \in V^m \mid \vec{v}\langle\vec{\tau}, \vec{x}\rangle \in f_j\}|. \quad (14)$$

Then

$$|\{\vec{x} \in V^{m+1} \mid \vec{v}\langle(\vec{\tau}, \tau_n), \vec{x}\rangle \in f_j\}| = \sum_{1 \leq s \leq c} \mu_{is} \lambda_{sj}.$$

which is clearly independent of the choice of \vec{v} within its equivalence class, by induction hypothesis and the fact that f is $C_{k,1}$ stable to start with. The result follows. \square

Corollary 5.4. *Any partition that is WL_k stable is also $C_{k,r}$ stable for all $r < k$.*

Proof. This is immediate since, as we noted above, WL_k stability implies C_k stability. \square

Remark 5.5. *Observe that if f is a WL_k stable partition of V^k refining atomic types, then the partition \bar{f} of V^{k-1} defined by $\bar{f}(\vec{x}) = f(\vec{x}, x_{k-1})$ is WL_{k-1} stable and refines atomic types.*

We are now in the position of proving Lemma 5.2.

Proof of Lemma 5.2. $WL_k(\iota^k)$ is a $C_{k,k-2}$ stable partition by Corollary 5.4. Call this partition ω for the sake of simplicity. Suppose $\omega(\vec{x}) = \omega(\vec{y})$. Then there is exactly one $\vec{z} \in V^{k-2}$ such that $\omega(\vec{y}\langle\vec{\tau}, \vec{z}\rangle) = \omega(\vec{x}\langle\vec{\tau}, \vec{z}\rangle)$ where $\tau = (r)_{r \in [k]}[i, j]$ and $\vec{z} = (x_i, x_i, x_i, \dots, x_i) \in V^{k-2}$. That is, for any $i, j \in [k]$, $\omega(\vec{x}) = \omega(\vec{y})$ implies that $\omega(\vec{x}') = \omega(\vec{y}')$ with

$$x'_r = \begin{cases} x_j & \text{for } r = j \\ x_i & \text{elsewhere} \end{cases} \quad (15)$$

and

$$y'_r = \begin{cases} y_j & \text{for } r = j \\ y_i & \text{elsewhere.} \end{cases} \quad (16)$$

As such, from Remark 5.5, (x_i, x_j) and (y_i, y_j) must be in the same equivalence class in \mathcal{R} . \square

Proof of Lemma 5.1. The fact that $\overline{\text{WL}}_j(\mathcal{R}) \preceq \overline{\text{WL}}_{j+1}(\mathcal{R})$ follows from Remark 5.5. Next we prove that $\overline{\text{WL}}_n(\mathcal{R})$ is indeed the Schurian of \mathcal{R} . In fact, let ψ be the colouring of V^r according to the orbits of the action of $\text{Aut}(W)$ on V^r , with $r \geq n$. Then this is a stable Weisfeiler-Leman partition, since

$$(\psi(\vec{v}), \sum_{x \in V} S_0(\vec{v}, x)) = (\psi(g \cdot \vec{v}), \sum_{x \in V} S_0(g \cdot \vec{v}, g \cdot x)) \quad (17)$$

for all $\vec{v} \in V^r$ and $g \in \text{Aut}(W)$. Furthermore, this is the coarsest partition refining $\eta^n(\mathcal{R})$. To see this we show that an refinement of $\eta^n(\mathcal{R})$ also refines ψ . Let ξ be some stable refinement of $\eta^n(\mathcal{R})$. First, note that for $r \geq n$ there are r -tuples $\vec{x}, \vec{y} \in V^r$ with exactly n distinct entries. As such, if $\xi(\vec{x}) = \xi(\vec{y})$, then the map $x_i \rightarrow y_i$ is the group action of an element $g \in \text{Aut}(W)$. Now, take any two $\vec{a}, \vec{b} \in V^r$ such that $\xi(\vec{a}) = \xi(\vec{b})$, and suppose \vec{a} and \vec{b} both have exactly s distinct entries in position i_1, \dots, i_s . Then there is some $\tau \in [r]^{(r-s)}$ with $\tau_j \neq i_l$ for all $j \in [r-s]$ and $l \in [s]$. As such, there are $\vec{x}, \vec{y} \in V^{r-s}$ with $n-s$ distinct entries and $x_i \neq y_j$ for all $i \in [r-s]$ and $j \in [r]$, satisfying $\xi(\vec{a} \langle \vec{\tau}, \vec{x} \rangle) = \xi(\vec{b} \langle \vec{\tau}, \vec{y} \rangle)$. Hence, there is some $g \in \text{Aut}(W)$ such that $g \cdot \vec{a} \langle \vec{\tau}, \vec{x} \rangle = \vec{b} \langle \vec{\tau}, \vec{y} \rangle$. Then it trivially follows that $g \cdot \vec{a} = \vec{b}$, hence $\psi(\vec{a}) = \psi(\vec{b})$ as required.

Also, for $j \leq k$, we have that $\overline{\text{WL}}_2(\overline{\text{WL}}_k(\mathcal{R})) = \overline{\text{WL}}_k(\mathcal{R})$. Note that $\overline{\text{WL}}_k(\overline{\text{WL}}_k(\mathcal{R})) = \overline{\text{WL}}_k(\mathcal{R})$, and hence $\overline{\text{WL}}_j(\overline{\text{WL}}_k(\mathcal{R})) \preceq \overline{\text{WL}}_k(\mathcal{R})$ by Remark 5.5. However, $\overline{\text{WL}}_k(\mathcal{R}) = \overline{\text{WL}}_2(\overline{\text{WL}}_k(\mathcal{R})) \preceq \overline{\text{WL}}_j(\overline{\text{WL}}_k(\mathcal{R})) \preceq \overline{\text{WL}}_k(\mathcal{R})$, and hence the result follows.

Finally, each of the k -Weisfeiler-Leman algorithms have a computational time of $n^{O(k)}$, so we have proven that they induce a Schurian polynomial approximation. \square

5.3 WL is equivalent to C

We now show a tight connection between the WL and C families. In particular, we want to establish Theorem 5.6 below, which is proved in [5, Section 5], but we formulate it in combinatorial terms (without reference to logic or games).

Recall that we write \equiv_{WL}^k for the equivalence relation corresponding to the partition $\text{WL}_k(\iota^k)$, i.e. the coarsest WL_k -stable partition that refines the partition into atomic types. Similarly, we write \equiv_C^k for the equivalence relation corresponding to $C_k(\iota^k)$. While these equivalence relations are defined on V^k , we also define them on V^j for all $j \in [k]$ by taking the j -projections of the induced partitions.

Theorem 5.6. *For each k on any graph, the partition induced by \equiv_{WL}^k is the same as that induced by \equiv_C^{k+1} .*

In order to prove this, we first show that a C_{k+1} -stable stable partition of V^{k+1} induces a natural WL_k -stable partition of V^k .

Lemma 5.7. *Let f and \bar{f} be partitions of V^{k+1} and V^k respectively refining atomic types. Suppose $\bar{f}(\vec{v}) = f(\vec{v}, v_k)$ for all $\vec{v} \in V^k$. Then \bar{f} is WL_k stable if f is C_{k+1} stable.*

Proof. Suppose f is C_{k+1} stable. Observe that for any $a, b \in V$,

$$f(\vec{x}, a) = f(\vec{y}, b) \implies \bar{f}(\vec{x}) = \bar{f}(\vec{y}). \quad (18)$$

Also note that

$$f(\vec{x}, a) = f(\vec{y}, b) \implies \bar{f}(\vec{x} \langle i, a \rangle) = \bar{f}(\vec{y} \langle i, b \rangle) \quad (19)$$

for all $i \in [k]$. Let Φ be the set of maps from $[k]$ to $\text{range}(f)$. Then the map $\delta_f : \text{range}(f) \rightarrow \Phi$ given by $\delta_f(f(\vec{x}, a)) = t$ with $t(i) = \bar{f}(\vec{x}\langle i, a \rangle)$ is well defined. It suffices to note that for any $t \in \Phi$

$$\{a \in V \mid \bar{f}(\vec{x}\langle i, a \rangle) = t(i) \forall i \in [k]\} = \{a \in V \mid \delta_f(f(\vec{x}, x_k))\langle k+1, a \rangle = t\}. \quad (20)$$

The size of the right hand side is independent of the choice of (\vec{x}, x_k) within its equivalence class by C_k equivalence, so the left hand side is also independent of the choice of representative of $\bar{f}(\vec{x})$ thus implying WL_k stability of \bar{f} . \square

Corollary 5.8. *For any graph G , and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_C^{k+1} \vec{v}$ implies $\vec{u} \equiv_{\text{WL}}^k \vec{v}$.*

Let $s \in \text{Sym}_k$ be a permutation of $[k]$. For any $\vec{v} \in V^k$ we define \vec{v}^s to have i^{th} entry equal to $v_{s(i)}$. Note that for WL_k and C_k partitions of V^k , \vec{u} and \vec{v} are in the same equivalence classes if and only if \vec{u}^s and \vec{v}^s are also in the same equivalence classes. As such, the equivalence class of \vec{x}^s may be denoted by $f(\vec{x}^s) = f(\vec{x})^s$. Also, for $t \in \Phi$, let t^s be such that $t^s(s(i)) = t(i)^s$. Furthermore, for $\vec{v} \in V^{k+1}$ denote $\vec{v}[i] = (v_1, v_2, \dots, v_{i-1}, v_{i+1}, \dots, v_{k+1}) \in V^k$.

Lemma 5.9. *Let \bar{f} be a WL_k stable partition of V^k and define a partition f of V^{k+1} as follows: $f(\vec{x}, a) = f(\vec{y}, b)$ if and only if $\bar{f}(\vec{x}) = \bar{f}(\vec{y})$ and $\bar{f}(\vec{x}\langle i, a \rangle) = \bar{f}(\vec{y}\langle i, b \rangle)$ for all $i \in [k]$. Then f is C_k stable.*

Proof. By the definition of WL_k stability, we see that for any $b, c \in V, \vec{y} \in V^{k+1}$ and $\vec{x} \in V^k$

$$\{a \in V \mid f((\vec{x}, b)\langle k+1, a \rangle) = f(\vec{x}, c)\} = \{a \in V \mid \bar{f}(\vec{x}\langle i, a \rangle) = t(i) \forall i \in [k]\} \quad (21)$$

where $t(i) = \bar{f}(\vec{x}\langle i, c \rangle)$. The size of the right hand side is independent of the choice of \vec{x} within $\bar{f}(\vec{x})$, and hence the left hand side is independent of the choice of $(\vec{x}, b) \in f(\vec{x}, b)$. We now note that for any $\vec{y} \in V^{k+1}$ the sequence

$$\bar{f}(\vec{y}[1]), \bar{f}(\vec{y}[2]), \bar{f}(\vec{y}[3]), \dots, \bar{f}(\vec{y}[k+1]) \quad (22)$$

is well defined and unique to each class of f . This is because there is some $s \in \text{Sym}_k$ such that for any $\vec{y} \in f(\vec{y})$ and $i \in [k]$, $\vec{y}[i] = \vec{y}[k+1]\langle i, y_{k+1} \rangle^s$. Hence, for all $\vec{y}, \vec{z} \in V^{k+1}$, the partition f may be equivalently defined as follows:

$$f(\vec{y}) = f(\vec{z}) \iff \bar{f}(\vec{y}[i]) = \bar{f}(\vec{z}[i]) \quad (23)$$

for any $i \in [k+1]$. As this definition is independent of $i \in [k+1]$, f can be equivalently defined as follows with arbitrary choice of $i \in [k+1]$ ¹:

$$f(\vec{y}) = f(\vec{z}) \iff \bar{f}(\vec{y}[i]) = \bar{f}(\vec{z}[i]) \text{ and } \bar{f}(\vec{y}[i]\langle j, y_{k+1} \rangle) = \bar{f}(\vec{z}[i]\langle j, z_{k+1} \rangle) \quad (24)$$

for all $j \in [k]$. Hence for all $\vec{x} \in V^{k+1}$ and $r \in [k+1]$.

$$\{a \in V \mid f((\vec{x})\langle r, a \rangle) = f(\vec{x}\langle r, c \rangle)\} = \{a \in V \mid \bar{f}(\vec{x}[r]\langle i, a \rangle) = t(i) \forall i \in [k]\} \quad (25)$$

where $t(i) = \bar{f}(\vec{x}[r]\langle i, c \rangle)$, and the result follows. \square

Corollary 5.10. *For any graph G , and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_{\text{WL}}^k \vec{v}$ implies $\vec{u} \equiv_C^{k+1} \vec{v}$.*

From this we get the result of Theorem 5.6 which, in the language of Schurian schemes, can be written as follows.

Corollary 5.11. *For any coherent configuration \mathcal{R} , $\overline{\text{WL}}_{k-1}(\mathcal{R}) = \overline{C}_k(\mathcal{R})$.*

In particular, the WL and C Schurian polynomial approximation schemes are equivalent in the sense of Definition 4.4.

¹We have obviously chosen $i = k+1$ in the statement of the proposition.

5.4 The width parameter r for WL and C

In Section 5.2 above, we introduced the width parameter, and the iterative refinement procedure $C_{k,r}$. This gives rise to an equivalence relation $\equiv_C^{k,r}$, which we define as the coarsest partition that refines ι^k and is $C_{k,r'}$ -stable for all $r' \in [r]$. The following is then immediate.

Theorem 5.12. *Let $\vec{u}, \vec{v} \in V^k$. For all $r < k$ the following holds:*

$$\vec{u} \equiv_C^k \vec{v} \iff \vec{u} \equiv_C^{k,r} \vec{v}. \quad (26)$$

Proof. The direction from left to right is immediate from the definition, while the other direction follows from Lemma 5.3. \square

In the proof above, the direction from left to right follows from the fact that in the definition of the equivalence $\equiv_C^{k,r}$ we allowed all widths $r' \in [r]$. If we only allowed width r , we get something weaker, as in the following lemma, which is a partial converse to Lemma 5.3.

Lemma 5.13. *Let f be a $C_{k,r}$ stable partition of V^k refining isomorphism types. Let g be the $k-r+1$ projection of f . Then g is a C_{k-r+1} stable partition.*

Proof. One simply needs to note that for all $\vec{x} \in V^{k-r+1}$, $i \in [k-r+1]$, $b \in V$, the following holds:

$$\{a \in V \mid g(\vec{x}\langle i, a \rangle) = g(\vec{x}\langle i, b \rangle)\} = \{a \in V \mid f((\vec{x}, x_{k-r+1}, x_{k-r+1}, \dots, x_{k-r+1})\langle \vec{\tau}, \vec{a} \rangle) = f((\vec{x}, x_{k-r+1}, x_{k-r+1}, \dots, x_{k-r+1})\langle \vec{\tau}, \vec{b} \rangle)\} \quad (27)$$

where $\vec{a} = (a, x_{k+r-1}, x_{k+r-1}, \dots, x_{k+r-1})$, $\vec{b} = (b, x_{k+r-1}, x_{k+r-1}, \dots, x_{k+r-1}) \in V^r$ and $\vec{\tau} = (i, r+1, r+2, \dots, k) \in [k]^{(k-r+1)}$. \square

Thus, the width parameter adds nothing to the family of algorithms C_k and yields an equivalent SPAS. As we see next, adding a width parameter to the WL scheme yields similar results. In contrast, with the IM scheme considered in Section 7, it is an open question whether the width parameter gives an equivalent scheme.

To formalise this for WL, we now define the refinement scheme $\{\text{WL}_{k,r}\}$.

- INPUT: a partition f_0 of V^k .
- OUTPUT: a partition f of V^k .
 1. Set $i = 0$.
 2. For all $\vec{v} \in V^k$ and $\vec{x} \in V^r$ define the vector

$$S_i(\vec{v}, \vec{x}) = (f_i(\vec{v}\langle \tau, x \rangle))_{\tau \in [k]^{(r)}} \quad (28)$$

Define also the formal sum

$$\sum_{\vec{x} \in V^r} S_i(\vec{v}, \vec{x}) \quad (29)$$

and set

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), \sum_{\vec{x} \in V^r} S_i(\vec{v}, \vec{x})). \quad (30)$$

3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ then output $f = f_i(\vec{v})$. Otherwise, repeat from step (2).

As before, we say that a f partition is $\text{WL}_{k,r}$ stable if $\text{WL}_{k,r}(f) = f$, and we write $\equiv_{\text{WL}}^{k,r}$ for the equivalence relation that is coarsest partition refining ι^k and that is $\text{WL}_{k,r'}$ -stable for all $r' \leq r$. We also use $\equiv_{\text{WL}}^{k,r}$ for the j -projections of this partition for $j \leq k$. It is immediate from the definition that if $\vec{u} \equiv_{\text{WL}}^{k,r} \vec{v}$, then $\vec{u} \equiv_{\text{WL}}^k \vec{v}$. In contrast to Theorem 5.12, we do not have a direct converse, but we can establish the following.

Lemma 5.14. *For any graph G , integers r, k with $r < k$ and $\vec{u}, \vec{v} \in V^k$, if $\vec{u} \equiv_{\text{WL}}^{k+r-1} \vec{v}$ then $\vec{u} \equiv_{\text{WL}}^{k,r} \vec{v}$.*

Proof. Let f be a C_{k+r} stable partition of V^{k+r} refining atomic types. Then the partition \bar{f} of V^k defined by $\bar{f}(\vec{x}) = f(\vec{x}, x_k, x_k, \dots, x_k)$ is $\text{WL}_{k,r}$ stable and refines atomic types. Indeed, the argument is analogous to that of Lemma 5.7, except that we substitute r -tuples into the first k positions of $k+r$ -tuples (as opposed to singlets into $(k+1)$ -tuples), and consider maps from $[k]^{(r)}$ to $\text{range}(\bar{f})$. \square

$\text{WL}_{k,r}$ stability trivially implies $C_{k,r}$ stability, and hence it holds that

Lemma 5.15. *For any graph G , integers r, k with $r < k$, and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_{\text{WL}}^{k,r} \vec{v}$ implies $\vec{u} \equiv_{\text{WL}}^{k-r} \vec{v}$.*

Proof. $\text{WL}_{k,r}$ stability trivially implies $C_{k,r}$ stability. The result then follows directly from Lemma 5.13 and the equivalence between C_{k+1} and WL_k . \square

As a consequence, we have the following.

Theorem 5.16. *The Schurian Polynomial Approximation Schemes given by WL_k , $\text{WL}_{k,r}$, C_k and $C_{k,r}$ are all equivalent. Indeed, for any $r, k \in \mathbb{N}$ with $r < k$*

- $\overline{\text{WL}}_k(\mathcal{R}) = \overline{C}_{k+1}(\mathcal{R})$.
- $\overline{C}_{k-r+1}(\mathcal{R}) \preceq \overline{C}_{k,r}(\mathcal{R}) \preceq \overline{C}_k(\mathcal{R})$.
- $\overline{\text{WL}}_{k-r}(\mathcal{R}) \preceq \overline{\text{WL}}_{k,r}(\mathcal{R}) \preceq \overline{\text{WL}}_{k+r-1}(\mathcal{R})$.

6 EP_k equivalence, quantum walks and strongly regular graphs

It is known by the result of Cai, Fürer and Immerman [5] that there is no fixed k such that \equiv_{WL}^k yields the partition into automorphism orbits on all graphs. By Theorem 5.16, this is also true of the other schemes we have so far considered. In the case of WL_2 , we already know that this fails to distinguish strongly regular graphs with the same parameters. We begin with a definition of strongly regular graphs.

Definition 6.1 (Strongly regular graph). *A graph is strongly regular if it is regular and there are integer parameters λ and μ such that:*

1. *every two adjacent vertices have λ common neighbours; and*
2. *every two non-adjacent vertices have μ common neighbours.*

It is still an open question as to whether there is a polynomial time algorithm for testing isomorphism for strongly regular graphs. It should be noted that the class of strongly regular graphs is not closed under disjoint unions. Thus, it is not immediately clear that the problems of isomorphism and of orbit partition are equivalent on this class. It has been conjectured that for some $k \in \mathbb{N}$ a member of the *Evdokimov-Ponomarenko* family of algorithms $\text{EP} = \{\text{EP}_k \mid k \in \mathbb{N}\}$ gives the automorphism partition on strongly regular graphs. Here we show that the scheme is equivalent (as an SPAS) to WL_k so the question is equivalent to asking if there is a k such that WL_k yields the automorphism partition on all strongly regular graphs. We begin with a definition of EP_k refinement.

- INPUT: A partition f_0 of V^{2k} .
- OUTPUT: A partition f of V^{2k} .

1. Set $i = 0$.
2. For all $\vec{v} \in V^{2k}$, let

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), \sum_{\vec{x} \in V^k} S_i(\vec{v}, \vec{x})) \quad (31)$$

where

$$S_i(\vec{v}, \vec{x}) = (f_i(\vec{v}\langle\vec{\tau}, \vec{x}\rangle), f_i(\vec{v}\langle\vec{\sigma}, \vec{x}\rangle)) \quad (32)$$

with $\vec{\tau} = (1, 2, 3, \dots, k) \in [2k]^{(k)}$ and $\vec{\sigma} = (k+1, k+2, k+3, \dots, 2k) \in [2k]^{(k)}$.

3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^{2k}$ output $f = f_i$. Else return to step (2).

The perceptive eye will note that all we are doing is executing WL_2 on pairs of elements of V^k . Thus the output f , which we indicate as $\text{EP}_k(f_0)$ is a coherent configuration over V^k . Let g be the coarsest WL_2 stable partition refining atomic types for some graph. For the purpose of graph isomorphism we take the following initial partition:

$$f_0^k(\vec{v}) = f_0^k(\vec{w}) \text{ if } \begin{cases} g(v, v) = g(w, w) & \text{if } \vec{v} = (v, v, \dots, v) \text{ and } \vec{w} = (w, w, \dots, w) \\ g(v_i, v_{i+k}) = g(w_i, w_{i+k}) \forall i \in [k] & \text{otherwise} \end{cases} \quad (33)$$

Showing that the refinements EP_k induce an SPAS is a bit more cumbersome then with WL_k , as EP_k is a partition of V^{2k} . For this purpose, the algebraic view of coherent configuration comes useful. Let \mathcal{R} be a coherent configuration and W its corresponding algebra. Recall that

$$\hat{W}^k = [W^{\otimes k}, I_\Delta]. \quad (34)$$

Observe that

$$\overline{W}^k = I_\Delta \hat{W}^k I_\Delta \quad (35)$$

is a well defined coherent configuration over V . Let $\overline{\mathcal{R}}_k$ be the coherent configuration corresponding to the algebra \overline{W}^k . We then let $\overline{\text{EP}}_k(\mathcal{R}) = \overline{\mathcal{R}}_k$. In [11] it is shown that for any coherent configuration \mathcal{R}

$$\overline{\text{WL}}_k(\mathcal{R}) \preceq \overline{\text{EP}}_k(\mathcal{R}) \preceq \overline{\text{WL}}_{3k}(\mathcal{R}). \quad (36)$$

In [11] it is shown that if g as in (33) above concides with some coherent configuration \mathcal{R} over V , then the equivalence classes of $\text{WL}_k(\eta^k(\mathcal{R}))$ are unions of cells of $\text{EP}_k(f_0^k)$. From this, it is easy to see the following.

Lemma 6.2. *Let $\vec{u}, \vec{v} \in V^k$. Then $\vec{u} \equiv_{\text{WL}}^k \vec{v}$ if $(\vec{u}, \vec{u}) \equiv_{\text{EP}}^k (\vec{v}, \vec{v})$.*

This shows the first inequality in (36). We can establish the other direction, but only up to a multiplicative factor.

Lemma 6.3. *Let $\vec{x}, \vec{y} \in V^{2k}$. Then $\vec{x} \equiv_{\text{EP}}^k \vec{y}$ if $\vec{x} \equiv_{\text{WL}}^{3k} \vec{y}$*

Proof. We prove this by showing that if f_0 is a partition of V^{2k} as in Equation 33, and f is a WL_{3k} stable partition refining atomic types, then the partition \bar{f} of V^{2k} defined as $\bar{f}(\vec{u}, \vec{v}) = f(\vec{u}, \vec{v}, v_k, v_k, \dots, v_k) \forall \vec{u}, \vec{v} \in V^k$, then \bar{f} is a refinement of $\text{EP}_k(f_0)$.

As f is WL_{3k} stable, it is also $C_{3k,k}$ stable and refines $\eta^{3k}(\mathcal{R}_G)$. We can view f as a C_3 stable partition of triples of k -tuples $(\vec{u}, \vec{v}, \vec{w})$. Hence, if viewed as a partition of pairs of k -tuples, \bar{f} is WL_2 stable and refines $\eta^{2k}(\mathcal{R}_G)$. It is clear that $\eta^{2k}(\mathcal{R}_G)$ is finer than f_0 . Since \bar{f} and $\text{EP}_k(f_0)$ both refine f_0 , are WL_2 stable partitions of pairs of k -tuples, and the latter is the coarsest of such, we must have that \bar{f} is finer than $\text{EP}_k(f_0)$ as required. \square

Going back to the discussion on strongly regular graphs, Lemma 6.3 shows that if for each $k \in \mathbb{N}$ we can construct a strongly regular CFI pair, then no EP_k is a perfect isomorphism test for strongly regular graphs. It would also be interesting to see whether it is true that if two graphs are not distinguished by the k -boson invariant (defined in Section 6.1 below), then they are not distinguished by $\text{EP}_{k'}$ for some $k' \in \mathbb{N}$. This could also shine some light on the complexity of isomorphism of strongly regular graphs.

We note that Evdokimov et al. [11] prove a similar result concerning Schurian polynomial approximation schemes. The above can be considered a stronger combinatorial version. Indeed, in [11], EP_k equivalence is discussed in terms of k -extended coherent algebras.

Definition 6.4 (k -extended coherent algebra). *Let W be a coherent algebra over V . We define its k -extension \hat{W}^k to be the coherent algebra over V^k defined as*

$$\hat{W}^k = [W^{\otimes k}, \Delta_I] \quad (37)$$

where

$$\Delta_I(\vec{u}, \vec{v}) = \begin{cases} 1 & \text{if } \vec{u} = \vec{v} = (u, u, \dots, u) \\ 0 & \text{elsewhere.} \end{cases} \quad (38)$$

Definition 6.5 (EP_k equivalence (algebraic version)). *Let G_1 and G_2 be graphs with adjacency matrices A_1 and A_2 respectively. We say that G_1 and G_2 are EP_k equivalent if there is some coherent algebra weak isomorphism $\hat{\phi} : [\hat{A}_1]^k \rightarrow [\hat{A}_2]^k$ such that*

1. $\hat{\phi}(X_1 \otimes \dots \otimes X_k) = \phi(X_1) \otimes \dots \otimes \phi(X_k)$ for some coherent algebra weak isomorphism $\phi : [A_1] \rightarrow [A_2]$ satisfying $\phi(A_1) = A_2$ and for all $X_i \in [A_1]$.
2. $\hat{\phi}(\Delta_I) = \Delta_{I'}$.

6.1 Quantum Walks

In [11], this algebraic treatment of EP_k is used to show that if two graphs are EP_k equivalent, then they share the same k -boson invariant. Consider a graph G with adjacency matrix A and a

quantum walk on G with Hamiltonian operator

$$\mathcal{H}_{kB} = -\frac{1}{k!} \left(\sum_{\sigma \in S_k} P_\sigma \right) A^{\oplus k} + \sum_{i \in [r]} U_i R_i. \quad (39)$$

We call the above the *Hamiltonian of the k -boson quantum walk on G* . The terms in the above are defined as follows:

1. $A^{\oplus k} = A \otimes I \otimes \dots \otimes I + I \otimes A \otimes \dots \otimes I + \dots + I \otimes I \otimes \dots \otimes A$.
2. $P_\sigma \vec{x} = (x_{\sigma(i)})_{i \in [k]} \forall \vec{x} \in V^k$.
3. For each tuple $\vec{x} \in V^k$ consider the following multiset:

$$V_{\vec{x}} = \{v_x \mid x \in V\} \quad (40)$$

where v_x is the number of $i \in [k]$ for which $x_i = x$. Partition V^k into equivalence classes Π_1, \dots, Π_r , where \vec{x} and \vec{y} are in the same equivalence class if and only if $V_{\vec{x}} = V_{\vec{y}}$. We then define

$$R_i \vec{x} = \begin{cases} \vec{x} & \text{if } \vec{x} \in \Pi_i \\ 0 & \text{otherwise.} \end{cases} \quad (41)$$

4. $U_i \in \mathbb{C}$.

Definition 6.6 (k -boson invariant). *For a graph G with adjacency matrix A , its k -boson invariant is defined to be the multiset of entries of the matrix $\exp(-i\mathcal{H}_{kB})$.*

In [17] it is shown that for any graph G with adjacency matrix A , $\exp(-i\mathcal{H}_{kB}) \in [\hat{A}]^k$. Furthermore, it is proven that any $\hat{\phi}$ witnessing a EP_k equivalence between two graphs, maps the k -boson Hamiltonian of one to the other. From Lemma 3.6 we can thus deduce that they share the same k -boson invariant.

7 Invertible maps

We now motivate the k -invertible map (IM_k) refinement as an attempt to strengthen C_k colouring schemes. These were first introduced with a different flavour by Dawar & Holm in [8].

7.1 Invertible maps over \mathbb{F}

Let $A = (A_1, A_2, \dots, A_r)$ be an array of $n \times n$ 01-matrices. Let

$$\mathcal{S}_{\mathbb{F}}(A) = \{X \in \text{Mat}_n(\{0, 1\})^r \mid \exists S \in GL_n(\mathbb{F}), SA_i S^{-1} = X_i \forall i \in [r]\}. \quad (42)$$

and define a total order on the set $[k]^{(2)}$ (say the standard lexicographic one).

Consider the following algorithm, the k -invertible map refinement over the field \mathbb{F} :

- INPUT: A partition f_0 of V^k .
- OUTPUT: A partition f of V^k .

1. Set $i = 0$.
2. Define a total order on the set $\text{range}(f_i)$. For each $\tau \in [k]^{(2)}$, $\vec{v} \in V^k$, and for each σ in the range of f_i let the boolean matrix $\chi_{\vec{v}, \tau}^\sigma$ labelled by V have (u, v) entry equal to 1 if and only if $f(\vec{v}_{\tau, (u, v)}) = \sigma$. For $\vec{v} \in V^k$ define $f_{i+1}(\vec{v}) = (f_i(\vec{v}), (\mathcal{S}_{\mathbb{F}}(X(\vec{\tau}, \vec{v})))_{\tau \in [k]^{(2)}})$ where $X(\vec{\tau}, \vec{v}) = (\chi_{\vec{v}, \tau}^\sigma)_{\sigma \in \text{range}(f_i)}$.
3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^k$ output the partition f_i . Otherwise, return to step 2.

In [15] the following result is proven.

Theorem 7.1. *Let $A = \{A_i \mid i \in I\}$ and $B = \{B_i \mid i \in I\}$ be classes of matrices over a field \mathbb{F} , and let \mathbb{K} be an extension of \mathbb{F} . Then A and B are simultaneously similar over \mathbb{F} if and only if they are simultaneously similar over \mathbb{K} . That is, there is an invertible matrix S over \mathbb{F} such that $SA_iS^{-1} = B_i$ for all $i \in I$ if and only if there is an invertible matrix T over \mathbb{K} such that $TA_iT^{-1} = B_i$.*

As every field of characteristic p contains a subfield isomorphic to \mathbb{Z}_p , we deduce that the above algorithm is independent of the field for a fixed characteristic. For any field \mathbb{F} , we write $\vec{u} \equiv_{\text{IM}}^{k, \mathbb{F}} \vec{v}$ to indicate that two tuples \vec{u} and \vec{v} of vertices in a graph are equivalent under the coarsest IM_k -stable partition over the field \mathbb{F} that refines ι^k .

We can claim that over characteristic 0, our understanding of the invertible map partitions is complete, as they can be understood in terms of Weisfeiler-Leman partitions. Indeed, the following hold.

Lemma 7.2. *For any graph G , and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_{\text{IM}}^{k, \mathbb{F}} \vec{v}$ implies $\vec{u} \equiv_{\text{WL}}^{k-2} \vec{v}$ over any field \mathbb{F} of characteristic 0.*

Proof. Given some partition f of V^k , observe that for any $\vec{v} \in V^k$, and $\vec{\tau} \in [k]^{(2)}$

$$\sum_{\sigma \in f} \chi_{\vec{v}, \vec{\tau}}^\sigma = J. \quad (43)$$

Thus, if $\vec{v} \equiv_{\text{IM}}^{k, \mathbb{C}} \vec{w}$, there is some S such that $SJS^{-1} = S$ and $S\chi_{\vec{v}, \vec{\tau}}^\sigma S^{-1} = \chi_{\vec{w}, \vec{\tau}}^\sigma$ for all colours σ and pairs $\vec{\tau} \in [k]^{(2)}$. We then deduce, using Lemma 3.7, that

$$|\{\vec{r} \in V^2 \mid f(\vec{v} \langle \vec{\tau}, \vec{r} \rangle) = \sigma\}| = |\{\vec{r} \in V^2 \mid f(\vec{w} \langle \vec{\tau}, \vec{r} \rangle) = \sigma\}|$$

and therefore $\vec{v} \equiv_C^{k, 2} \vec{w}$. The desired result follows from Theorem 5.16 □

Lemma 7.3. *For any graph G and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_{\text{WL}}^k \vec{v}$ implies $\vec{u} \equiv_{\text{IM}}^{k, \mathbb{C}} \vec{v}$.*

Proof. It is sufficient to show that: if f is a C_{k+1} stable partition of V^{k+1} refining atomic types, then the partition \bar{f} of V^k defined as $\bar{f}(\vec{x}) = f(\vec{x}, x_k)$ is IM_k stable.

Define f' to be the partition of V^{k+1} with $f'(\vec{v}) = f'(\vec{w})$ if and only if $f(\vec{v}) = f(\vec{w})$ or $v_i = w_i$ for all $i \in [k]$. It can be shown that f' is also a C_{k+1} stable partition (though note that it does not refine atomic types). Observe that if we define \bar{f} as $\bar{f}(\vec{v}[k+1]) = f(\vec{v})$, then \bar{f} is a well defined C_k partition of V^k refining atomic types. Now, fix some $\vec{v} \in V^{k+1}$ and $\vec{\tau} \in [k]^{(3)}$ with $\tau_3 = k+1$.

Let g_v be the partition of V^3 defined as $g_v(\vec{u}) = f(\vec{v}(\vec{\tau}, \vec{u}))$. Let us define g'_v and \bar{g}_v in terms of g_v analogously to f' and \bar{f} in terms of f . That is:

$$g'_v(\vec{u}) = g'_v(\vec{w}) \text{ if } g_v(\vec{u}) = g_v(\vec{w}) \text{ or } u_i = w_i \forall i \in \{1, 2\}, \forall \vec{u}, \vec{w} \in V^3. \quad (44)$$

and

$$\bar{g}_v(\vec{u}[3]) = g'_v(\vec{u}) \forall \vec{u} \in V^3. \quad (45)$$

Then since g'_v is a C_3 stable partition of V^3 , \bar{g}_v is a coherent configuration over V by Corollary 5.6. Furthermore, if $\bar{f}(\vec{v}) = \bar{f}(\vec{w})$, then \bar{g}_v and \bar{g}_w are weakly isomorphic coherent configurations. The result then follows from Lemma 3.6. \square

Note that the discrepancy between $C_{k,r}$ and $WL_{k,r}$ is that the former classifies k -tuples by inducing a partition on V^r for each $\vec{\tau} \in [k]^{(r)}$. That is, for each $\vec{\tau} \in [k]^{(r)}$ and $\vec{x} \in V^r$ we have a partition of V^r given by $\pi_{\vec{\tau}}(\vec{x}) = f(\vec{v}(\vec{\tau}, \vec{x}))$. The latter, instead, classifies k -tuples by considering the coarsest partition of V^r refining $\pi_{\vec{\tau}}$ for all $\vec{\tau} \in [k]^{(r)}$. Let us stick to the case $m = 1$ for the sake of our discussion. In a similar way, IM_k classifies k -tuples by considering partitions of V^2 for each $\vec{\tau} \in [k]^{(2)}$, which give rise to the matrices $\chi_{\vec{v}, \vec{\tau}}^\sigma$. Consider the following algorithm, which we shall label as IM'_k over the field \mathbb{F} .

- INPUT: A partition f_0 of V^k .
 - OUTPUT: A partition f of V^k .
1. Set $i = 0$.
 2. Define a total order on the set T_i of maps from $[k]^{(2)}$ to $range(f_i)$. For each $\vec{v} \in V^k$ and $t \in T_i$, define the $V \times V$ matrix $\chi_{\vec{v}}^t$ to have (u, v) entry equal to 1 if $f_i(\vec{v}(\langle i, j \rangle, (u, v))) = t(i, j)$ for all $(i, j) \in [k]^{(2)}$. Let $f_{i+1}(\vec{v}) = (f_i(\vec{v}), \mathcal{S}_{\mathbb{F}}(X))$ where $X = (\chi_{\vec{v}}^t)_{t \in T_i}$.
 3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^k$ output f_i . Otherwise, return to step 2.

Observe that $\chi_{\vec{v}}^t$ is simply the Schur-Hadamard product of all matrices $\chi_{\vec{v}, (i, j)}^\sigma$ where $\sigma = t(i, j)$.

It is trivial to see that for any field \mathbb{F} and $\vec{u}, \vec{v} \in V^k$ it is true that

$$\vec{u} \equiv_{IM'}^{k, \mathbb{F}} \vec{v} \implies \vec{u} \equiv_{IM}^{k, \mathbb{F}} \vec{v}.$$

Also, in the same way $\vec{u} \equiv_C^{k+1} \vec{v} \implies \vec{u} \equiv_{WL}^k \vec{v}$, we have that

Corollary 7.4. *For any graph G , field \mathbb{F} and $\vec{u}, \vec{v} \in V^k$, $\vec{u} \equiv_{IM}^{k+2, \mathbb{F}} \vec{v}$ implies $\vec{u} \equiv_{IM'}^{k, \mathbb{F}} \vec{v}$.*

which is a direct consequence of the following result.

Lemma 7.5. *Let f be a IM_{k+2} stable partition of V^{k+2} refining atomic types. Let \bar{f} be a partition of V^k defined as $\bar{f}(\vec{v}) = f(\vec{v}, v_k, v_k)$ for all $\vec{v} \in V^k$. Then \bar{f} is a IM'_k stable partition refining atomic types.*

Proof. The argument is essentially analogous to that of Lemma 5.7.

Observe that if f is IM_k stable refining atomic types, then for all $\vec{u}, \vec{v} \in V^k$ and $\vec{x}, \vec{y} \in V^2$

$$f(\vec{u}, \vec{x}) = f(\vec{v}, \vec{y}) \implies \bar{f}(\vec{u}) = \bar{f}(\vec{v}). \quad (46)$$

In addition, the map $\delta_f : \text{range}(f) \rightarrow \Phi$ given by

$$\delta_f(f(\vec{x}, \vec{y})(\vec{\tau})) = \bar{f}(\vec{v}(\vec{\tau}, \vec{y})) \quad (47)$$

is well defined for all $\vec{x} \in V^k, \vec{y} \in V^2, \tau \in [k]^{(2)}$ and Φ being the set of maps from $[k]^{(2)}$ to $\text{range}(\bar{f})$. Now, for all $t \in \Phi, \vec{v} \in V^k$, we have that

$$\chi_{\vec{v}}^t = \sum_{\sigma \in \text{range}(f) | \delta_f(\sigma) = t} \chi_{(k+1, k+2), \vec{v}}^\sigma \quad (48)$$

The statement of this Lemma then follows directly from the linearity of the map $X \rightarrow SXS^{-1}$. \square

We do not expect a converse to this to hold. Indeed, some careful consideration would reveal that it is not possible to replicate the argument of Lemma 5.9 in this case.

Of course, the algorithms IM_k and IM'_k can be embedded into the concept of Schurian schemes, again, by considering the 2-projection of the output partitions, \overline{IM}_k and \overline{IM}'_k respectively. Before formulating the above results in the language of Schurian schemes, we make this small modification to the above algorithms:

- In step 2 of algorithm IM_k we replace the definition of f_{i+1} by the following new one:

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), (\mathcal{S}_{\mathbb{F}}(X(\vec{\tau}, \vec{v})))_{\tau \in [k]^{(2)}}, \sum_{x \in V} S_i(\vec{v}, x)) \quad (49)$$

where the formal sum $\sum_{x \in V} S_i(\vec{v}, x)$ is as in equation 6.

- Likewise, in step 2 of algorithm IM'_k we replace the definition of f_{i+1} by the following:

$$f_{i+1}(\vec{v}) = (f_i(\vec{v}), \mathcal{S}_{\mathbb{F}}(X), \sum_{x \in V} S_i(\vec{v}, x)). \quad (50)$$

In other words, the equivalence between tuples has to be witnessed both by invertible matrices and k -Weisfeiler-Leman equivalence. This is a rather important modification as it allows us to regain combinatorial properties which may be lost from the algebraic definition. Also, this restriction is done without loss of generality: indeed, for $\text{char}(\mathbb{F}) = 0$, the \overline{IM} Schurian Scheme is essentially equivalent to \overline{WL} , and for $\text{char}(\mathbb{F}) > 0$ it can be argued that \overline{IM} improves \overline{WL} (see Section 7.2). With this new definitions in mind, we can state as follows.

Proposition 7.6. *For fields of characteristic 0, the Schurian polynomial approximations given by WL_k and IM_k are equivalent. In particular, for $k \in \mathbb{N}$, and any coherent configuration \mathcal{R} , we have that*

$$\overline{IM}_k(\mathcal{R}) = \overline{WL}_k(\mathcal{R}). \quad (51)$$

Remark 7.7. *For IM_k to give a SPAS we need the algorithm to run in polynomial time: indeed, simultaneous similarity can be tested in polynomial time over any field, as shown in [4].*

Remark 7.8. *Suppose on some graph G , IM'_k outputs the partition into automorphism orbits of V^k . Then, the matrices witnessing the equivalence $\vec{u} \equiv_{\overline{IM}}^{k, \mathbb{F}} \vec{v}$ for some $\vec{u}, \vec{v} \in V^k$ can be taken to be a permutation matrix of the automorphism group of G . That is, if for all $t \in T$, where T is the set of maps from $[k]^{(2)}$ to the colours of the stable partition, there is an $S \in GL_V(\mathbb{F})$, we have $S\chi_{\vec{v}}^t S^{-1} = \chi_{\vec{u}}^t$, then S can be taken to be the permutation matrix corresponding to the action of some element of $\text{Sym}(V)$.*

7.2 Further extensions of IM_k and open questions

The previous section settled the question about the power of the invertible map scheme on fields of characteristic 0. As a Schurian polynomial approximation scheme it is equivalent to the various others we have studied, including the Weisfeiler-Leman scheme. It is over fields of positive characteristic that this scheme is more powerful. This is summed up in the following proposition.

Proposition 7.9. *IM improves WL.*

Proof. For any $k \in \mathbb{N}$, prime p and coherent configuration \mathcal{R} , over \mathbb{Z}_p $\overline{\text{WL}}_{k-2}(\mathcal{R}) \preceq \overline{\text{IM}}_k(\mathcal{R})$. This follows by an argument similar to the proof of Lemma 7.2. In particular, we show that for any partition of V^{k-1} whose 2-projection is a coherent configuration, if it is IM_k -stable it is also C_{k-1} -stable. Thus, suppose that f is an IM_k -stable partition of V^{k-1} and \bar{f} is a coherent configuration. In particular, this means that if two k -tuples \vec{a} and \vec{b} are in the same colour of f , then $a_i = a_j$ if, and only if, $b_i = b_j$ for any $i, j \in [k]$. Now, let \vec{v} and \vec{w} be two tuples in the same colour of f and let σ be an arbitrary colour. Let \vec{v}' and \vec{w}' be the k -extensions of these two tuples. Hence, there is an S such that for any $\tau \in [k]^{(2)}$, and any part ρ of f , we have $S\chi_{\vec{v}',\tau}^\rho S^{-1} = \chi_{\vec{w}',\tau}^\rho$. In particular, consider τ to be the pair (i, k) for some $i < k$ and σ' to be the unique colour in the k -lift of f whose restriction to $[k-1]$ is σ and such that $\vec{u} \in \sigma'$ implies $u_i = u_k$. Then, $\chi_{\vec{v}',\tau}^{\sigma'}$ and $\chi_{\vec{w}',\tau}^{\sigma'}$ only have non-zero entries in the diagonal. Since, $S\chi_{\vec{v}',\tau}^{\sigma'} S^{-1} = \chi_{\vec{w}',\tau}^{\sigma'}$, the two matrices have the same rank and therefore the same number of non-zero entries. It follows that $|\{x \mid \vec{v} < i, x > \in \sigma\}| = |\{x \mid \vec{w} < i, x > \in \sigma\}|$, and therefore the partition is C_{k-1} -stable.

To show that WL does not simulate IM over \mathbb{Z}_2 , it suffices to note that IM_3 distinguishes the Cai-Fürer-Immerman graphs, as noted in [8]. Similarly, for characteristic p other than 2, the construction by Holm [14] of CFI graphs in characteristic p which can be distinguished in IM_3 of characteristic p establishes this. \square

The proof relies on the construction, given in Holm's thesis [14] of generalized CFI graphs over any characteristic p . Indeed, it is shown there that for each p and k , we can construct such a pair of graphs G and H which are distinguished by IM_3 over \mathbb{Z}_p but not by IM_k over \mathbb{Z}_q for any $q \neq p$. A consequence of this is that there is no fixed p and k such that $\equiv_{\text{IM}}^{k, \mathbb{Z}_p}$ gives a test for isomorphism on all graphs. Indeed, for any set of primes Q , define $\equiv_{\text{IM}}^{k, Q}$ to be the coarsest common refinement of $\equiv_{\text{IM}}^{k, \mathbb{Z}_p}$ for all $p \in Q$. Then, the result implies that as long as Q is not the set of all primes, there is no k such that $\equiv_{\text{IM}}^{k, Q}$ yields a test for isomorphism.

We can further strengthen the IM scheme by adding a width parameter, just as we did in the case of C and WL. Formally, we define the IM_k^m refinement over a field \mathbb{F} by the following algorithm.

- INPUT: A partition f_0 of V^k .
 - OUTPUT: A partition f of V^k .
1. Set $i = 0$.
 2. Define a total order on the set $\text{range}(f_i)$. For each $\tau \in [k]^{(2m)}$, $\vec{v} \in V^k$, and for each σ in the range of f_i let the boolean matrix $\chi_{\vec{v},\tau}^\sigma$ labelled by V^m have (\vec{u}, \vec{v}) entry equal to 1 if and only if $f(\vec{v}_\tau, (\vec{u}, \vec{v})) = \sigma$. For $\vec{v} \in V^k$ define $f_{i+1}(\vec{v}) = (f_i(\vec{v}), (\mathcal{S}_{\mathbb{F}}(X(\vec{\tau}, \vec{v})))_{\tau \in [k]^{(2m)}}$ where $X(\vec{\tau}, \vec{v}) = (\chi_{\vec{v},\tau}^\sigma)_{\sigma \in \text{range}(f_i)}$.

3. If $f_{i+1}(\vec{v}) = (f_i(\vec{v}), f_i(\vec{v}))$ for all $\vec{v} \in V^k$ output the partition f_i . Otherwise, return to step 2.

As before, we define the equivalence relation $\equiv_{\text{IM}}^{k,m,\mathbb{F}}$ as the coarsest partition that refines ι_k and is $\text{IM}_{k,m'}$ -stable over \mathbb{F} for all $m' \in [m]$. In contrast to the results we obtained for C and WL, it is an open question whether IM_k can simulate IM_k^m . On the other hand, we do know that even for the relations $\equiv_{\text{IM}}^{k,m,\mathbb{F}}$, it is important to have fields of all characteristics. In particular, a recent result of Dawar et al. [9] has shown that for each prime p and integers k, r with $2m < k$, we can construct such a pair of graphs G and H which are not distinguished by IM_k^m over \mathbb{Z}_q for any $q \neq p$.

8 Conclusions

The Weisfeiler-Leman algorithm is much studied in the context of graph isomorphism. It is really a family of algorithms, graded by a dimension parameter. A large number of other families of algorithms have been shown to give essentially the same graded approximations of isomorphism. The Schurian polynomial approximation schemes of Evdokimov et al. provide a general framework for comparing these families of algorithms.

The subtle difference between the Weisfeiler-Leman family (WL) and the counting family (C) is based on tuple-based versus position-based refinement. This is known to lead to a difference of 1 in the dimension (i.e. C_{k+1} is equivalent to WL_k) though the two give equivalent schemes. The difference is somewhat amplified when we add the width parameter, but as we showed, we still get equivalent SPAS. We also showed equivalence with the EP scheme introduced by Braghi and Ponomarenko.

The invertible map schemes of Dawar and Holm provide another variation. In addition to the dimension k , they have two further parameters, the width, and the characteristic of the fields considered. We know that the width 1, characteristic 0 case gives a SPAS equivalent to WL_k . We also showed that this remains true if we strengthen the scheme to allow tuple-wise refinement. We know that the scheme with positive characteristic is strictly more powerful. The effect of the width parameter remains an open question.

For future work, it would be useful to include other graded approximations of isomorphism that have been studied in the literature, and study them within this same framework. One particular one of interest is the scheme introduced by Derksen [10] which, like the IM scheme is parameterised by a field.

References

- [1] A. Atserias and E. N. Maneva. Sherali-Adams relaxations and indistinguishability in counting logics. *SIAM J. Comput.*, 42:112–137, 2013.
- [2] L. Babai. Graph isomorphism in quasipolynomial time [extended abstract]. In *Proc. 48th Annual ACM SIGACT Symp. Theory of Computing, STOC*, pages 684–697, 2016.
- [3] Peter A. Brooksbank and Eugene M. Luks. Testing isomorphism of modules. *Journal of Algebra*, 320(11):4020 – 4029, 2008. Computational Algebra.
- [4] J. Y. Cai, M. Fürer, and N. Immerman. An optimal lower bound on the number of variables for graph identification. *Combinatorica*, 12(4):389–410, Dec 1992.

- [5] P. Cameron. *Permutation groups*. Cambridge University Press, 1999.
- [6] P. Cameron. Coherent configurations, association schemes and permutation groups. *Groups, Combinatorics and Geometry*, 10 2001.
- [7] A. Dawar and B. Holm. Pebble games with algebraic rules. *Fundam. Inform.*, 150(3-4):281–316, 2017.
- [8] Anuj Dawar, Erich Grädel, and Wied Pakusa. Approximations of isomorphism and logics with linear-algebraic operators. arxiv 1902.06648, 2019.
- [9] Harm Derksen. The graph isomorphism problem and approximate categories. *Journal of Symbolic Computation*, 59:81 – 112, 2013.
- [10] S. Evdokimov, M. Karpinsky, and I. Ponomarenko. On a new high dimensional weisfeiler-lehman algorithm. *Journal of Algebraic Combinatorics*, 10, July 1999.
- [11] S. Friedland. Coherent algebras and the graph isomorphism problem. *Discrete Applied Mathematics*, 25(1):73 – 98, 1989.
- [12] Lauri Hella. Logical hierarchies in ptime. *Information and Computation*, 129(1):1 – 19, 1996.
- [13] B. Holm. *Descriptive complexity of linear algebra*. PhD thesis, University of Cambridge, 2010.
- [14] L. Klingler and L. S. Levy. Sweeping-similarity of matrices. *Linear Algebra and its Applications*, 75:67 – 104, 1986.
- [15] P. N. Malkin. Sherali-Adams relaxations of graph isomorphism polytopes. *Discrete Optimization*, 12:73–97, 2014.
- [16] J. Smith. *Algebraic aspects of Multi-Particle Quantum Walks*. PhD thesis, University of Waterloo, 2012.
- [17] B. Yu. Weisfeiler. *On construction and identification of graphs*. Springer-Verlag Berlin Heidelberg, 1976.