Local WL Invariance and Hidden Shades of Regularity

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Abstract

The k-dimensional Weisfeiler-Leman algorithm is a powerful tool in graph isomorphism testing. For an input graph G, the algorithm determines a canonical coloring of s-tuples of vertices of G for each s between 1 and k. We say that a numerical parameter of s-tuples is k-WL-invariant if it is determined by the tuple color. As an application of Dvořák's result on k-WL-invariance of homomorphism counts, we spot some non-obvious regularity properties of strongly regular graphs and related graph families. For example, if G is a strongly regular graph, then the number of paths of length 6 between vertices x and y in G depends only on whether or not x and y are adjacent (and the length 6 is here optimal). Or, the number of cycles of length 7 passing through a vertex x in G is the same for every x (where the length 7 is also optimal).

1 Introduction

The k-dimensional Weisfeiler-Leman algorithm (k-WL) is a powerful combinatorial tool for detecting non-isomorphism of two given graphs. Playing a constantly significant role in isomorphism testing, it was used, most prominently, in Babai's quasipolynomial-time isomorphism algorithm [2].

For each k-tuple $\bar{x} = (x_1, \ldots, x_k)$ of vertices in an input graph G, the algorithm computes a canonical color $WL_k(G, \bar{x})$; see the details in Section 2. If the multisets of colors $\{\!\!\{WL_k(G, \bar{x}) : \bar{x} \in V(G)^k\}\!\!\}$ and $\{\!\!\{WL_k(H, \bar{y}) : \bar{y} \in V(H)^k\}\!\!\}$ are different for two graphs G and H, then these graphs are clearly non-isomorphic, and we say that k-WL distinguishes them. If k-WL does not distinguish G and H, we say that these graphs are k-WL-equivalent and write $G \equiv_{k-WL} H$. As proved by Cai, Fürer, and Immerman [6], the k-WL-equivalence for any fixed dimension k is strictly coarser than the isomorphism relation on graphs. For k = 2, an example of two non-isomorphic 2-WL-equivalent graphs is provided by any pair of non-isomorphic strongly regular graphs with the same parameters. The smallest such pair consists

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Figure 1: The Shrikhande graph S drawn on a torus; vertices of the same color form 4-cycles (some edges are not depicted). Though both a, a' and b, b' are non-adjacent, the common neighbors of a and a' are non-adjacent, while the common neighbors of b and b' are adjacent. The automorphism group of S acts transitively on the ordered pairs of non-adjacent vertices of each type [20].

of the Shrikhande and the 4×4 rook's graphs. The Shrikhande graph, which will occur several times in the sequel, is the Cayley graph of the abelian group $\mathbb{Z}_4 \times \mathbb{Z}_4$ with connecting set $\{(1,0), (0,1), (1,1)\}$. Figure 1 shows a natural drawing of this graph on the torus.

Let $\hom(F, G)$ denote the number of homomorphisms from a graph F to a graph G. A characterization of the k-WL-equivalence in terms of homomorphism numbers by Dvořák [10] implies that the homomorphism count $\hom(F, \cdot)$ is k-WL-invariant for each pattern graph F of treewidth at most k, that is, $\hom(F, G) = \hom(F, H)$ whenever $G \equiv_{k-WL} H$.

Let $\operatorname{sub}(F, G)$ denote the number of subgraphs of G isomorphic to F. Lovász [17, Section 5.2.3] showed a close connection between the homomorphism and the subgraph counts, which found many applications in various context. Curticapean, Dell, and Marx [9] used this connection to design efficient algorithms for counting the number of F-subgraphs in an input graph G. In [1], we addressed WL invariance of the subgraph counts. Define the homomorphism-hereditary treewidth htw(F) of a graph F as the maximum treewidth of the image of F under an edge-surjective homomorphism. Then Dvořák's invariance result for homomorphism counts, combined with the Lovász relationship, implies that $\operatorname{sub}(F, G) = \operatorname{sub}(F, H)$ whenever $G \equiv_{k-WL} H$ for k = htw(F).

In fact, Dvořák [10] proves his result in a stronger, *local* form. To explain what we here mean by locality, we need some additional technical concepts. A graph F with s designated vertices z_1, \ldots, z_s is referred to as s-labeled. A tree decomposition and the treewidth of (F, \bar{z}) are defined as usually with the additional requirement that at least one bag of the tree decomposition must contain all z_1, \ldots, z_s .¹ A homomorphism from an s-labeled graph (F, z_1, \ldots, z_s) to an s-labeled graph (G, x_1, \ldots, x_s) must take z_i to x_i for every $i \leq s$. Denote the number of such homomorphisms by hom $(F, \bar{z}; G, \bar{x})$.

The canonical coloring of the Cartesian power $V(G)^k$ produced by k-WL deter-

¹Imposing this condition is equivalent to the recursive definition given in [10].

mines a canonical coloring of $V(G)^s$ for each s between 1 and k. Specifically, if s < k, we define $WL_k(G, x_1, \ldots, x_s) = WL_k(G, x_1, \ldots, x_s, \ldots, x_s)$ just by cloning the last vertex in the s-tuple k - s times. Dvořák [10] proves that, if an s-labeled graph (F, \bar{z}) has treewidth k, then even local homomorphism counts hom $(F, \bar{z}; \cdot)$ are k-WL-invariant in the sense that hom $(F, \bar{z}; G, \bar{x}) = hom(F, \bar{z}; H, \bar{y})$ whenever k-WL assigns the same color to the s-tuples \bar{x} and \bar{y} , i.e., $WL_k(G, \bar{x}) = WL_k(H, \bar{y})$.

Our first observation is that, like for ordinary unlabeled graphs, this result can be extended to local subgraph counts. Given a pattern graph F with labeled vertices z_1, \ldots, z_s and a host graph G with labeled vertices x_1, \ldots, x_s , we write $\operatorname{sub}(F, \overline{z}; G, \overline{x})$ to denote the number of subgraphs S of G with $x_1, \ldots, x_s \in V(S)$ such that there is an isomorphism from F to S mapping z_i to x_i for all $i \leq s$. The local subgraph counts $\operatorname{sub}(F, z_1, \ldots, z_s; \cdot)$ are k-WL-invariant for $k = htw(F, \overline{z})$, where the concept of the homomorphism-hereditary treewidth is extended to s-labeled graphs in a straightforward way. That is, not only the k-WL-equivalence type of G determines the total number of F-subgraphs in G, but even the color $\operatorname{WL}_k(G, x_1, \ldots, x_s)$ of each s-tuple of vertices determines the number of extensions of this particular tuple to an F-subgraph (see Lemma 3.3).

Consider as an example the pattern graph $F = P_6$ where P_6 is a path through 6 vertices z_1, \ldots, z_6 . Consider also two host graphs R and S where R is the 4×4 -rook's graph, and S is the Shrikhande graph. Since $htw(P_6) = 2$, the "global" invariance result in [10] implies that R and S contain equally many 6-paths. Indeed, $sub(P_6, R) = sub(P_6, S) = 20448$.

Moreover, we have $htw(P_6, z_1, z_6) = 2$; see Figure 2a. It follows that the count $sub(P_6, z_1, z_6; G, x, x')$ is determined by $WL_2(G, x, x')$ for every graph G and every pair of vertices x, x' in G. If G is a strongly regular graph, then $WL_2(G, x, x')$ depends only on the parameters of G and on whether x and x' are equal, adjacent, or non-adjacent. Applied to $G \in \{R, S\}$, this justifies the fact that $sub(P_6, z_1, z_6; R, x, x') = sub(P_6, z_1, z_6; S, y, y') = 156$ for every pair of adjacent vertices x, x' in R and every pair of adjacent vertices y, y' in S. If x and x' as well as y and y' are not adjacent, then $sub(P_6, z_1, z_6; R, x, x') = sub(P_6, z_1, z_6; R, x, x') = sub(P_6, z_1, z_6; R, x, x') = sub(P_6, z_1, z_6; S, y, y') = 180.$

Note that the condition $htw(P_6, z_1, z_6) = 2$ is essential here. Indeed, the slightly modified pattern (P_6, z_2, z_5) does not enjoy anymore the above invariance property. For example, for the two vertex pairs a, a' and b, b' in Figure 1 we have $sub(P_6, z_2, z_5; S, a, a') = 244$ while $sub(P_6, z_2, z_5; S, b, b') = 246$, even though both pairs are non-adjacent. The difference between the patterns (P_6, z_1, z_6) and (P_6, z_2, z_5) , is explained by the fact that $htw(P_6, z_2, z_5) = 3$; see Figure 2b.

As we have seen, the number of 6-paths between two vertices is the same for any two adjacent (resp., non-adjacent) vertices in R and in S. The same holds true also for 7-paths and for any strongly regular graph. This general fact follows from the 2-WL-invariance of the subgraph counts for P_s with labeled end vertices for $s \leq 7$ and from the fact that, if G is a strongly regular graph, then the color $WL_k(G, x, x')$ is the same for all adjacent and all non-adjacent pairs x, x'. Our main purpose in this note is to collect such non-obvious regularity properties, which are not directly implied by the definition of a strongly regular graph; see Theorem

Figure 2: (a) Homomorphic images of (P_6, z_1, z_6) up to isomorphism and root swapping. (b) (P_6, z_2, z_5) and its image under the homomorphism h which maps z_1 to z_4 , z_6 to z_3 , and fixes all other vertices. Since $h(z_2)$ and $h(z_5)$ must be in one bag, the homomorphism-hereditary treewidth increases to 3.

4.1. As a further example of implicit regularity, the number of 7-cycles containing a specified edge in a strongly regular graph does not depend on the choice of this edge. This is actually true for a larger class of graphs, namely for constituent graphs of association schemes, in particular, for all distance-regular graphs; see Theorem 4.3. Also, the number of 7-cycles passing through a specified vertex in a strongly regular graph does not depend on the choice of this vertex. The last property also holds true for constituent graphs of association schemes and even for a yet larger class of WL_{1,2}-regular graphs [11]; see Theorem 4.4.

Related work. Godsil [13] proves that, if G is a constituent graph of an association scheme, then the number of spanning trees containing a specified edge of G is the same for every choice of the edge. Note that this "local" result also has a "global" invariance analog. If two graphs G and H are 2-WL-equivalent, then they have the same number of spanning trees. This follows from Kirchhoff's theorem because 2-WL-equivalent graphs are cospectral [12].

2 Formal definitions

Graph-theoretic preliminaries. The vertex set of a graph G is denoted by V(G). A graph G is *s*-regular if every vertex of G has exactly *s* neighbors. An *n*-vertex *s*-regular graph G is *strongly regular* with parameters (n, s, λ, μ) if every two adjacent vertices of G have λ common neighbors and every two non-adjacent vertices have μ common neighbors. The Shrikhande and the 4×4 rook's graphs, which were mentioned in Section 1, have parameters (16, 6, 2, 2).

A tree decomposition of a graph G is a tree T and a family $\mathcal{B} = \{B_i\}_{i \in V(T)}$ of sets $B_i \subseteq V(G)$, called bags, such that the union of all bags covers all V(G), every edge of G is contained in at least one bag, and we have $B_i \cap B_j \subseteq B_l$ whenever l lies on the path from i to j in T. The width of the decomposition is equal to $\max |B_i| - 1$. The treewidth of G, denoted by tw(G), is the minimum width of a tree decomposition of G. Moreover, we define htw(G), the homomorphism-hereditary treewidth of G, as the maximum tw(H) over all graphs H such that there is an edge-surjective homomorphism from G to H. We give a simple example for further reference.

Example 2.1. $htw(C_s) = 2$ for $3 \le s \le 7$, where C_s denotes the cycle graph on s vertices. Indeed, a simple inspection shows that, if $s \le 7$, then all edge-surjective homomorphic images of C_s are outerplanar graphs with one exception for the graph formed by three triangles sharing a common edge, which is an image of C_7 . Another argument, based on a characterization of the class of all graphs with homomorphism-hereditary treewidth at most 2, can be found in [1]. Since this class is closed under taking subgraphs, we also have $htw(P_s) = 2$ for $s \le 7$.

The Weisfeiler-Leman algorithm. The original version of the algorithm, 2-WL, was described by Weisfeiler and Leman in [21]. For an input graph G, this algorithm assigns a color to each pair of vertices (x, y) and then refines the coloring of the Cartesian square $V(G)^2$ step by step. Initially, $WL_2^0(G, x, y)$ is one of three colors depending on whether x and y are adjacent, non-adjacent, or equal. The coloring after the *i*-th refinement step, $WL_2^i(G, x, y)$, is computed as

$$WL_{2}^{i}(G, x, y) = (WL_{2}^{i-1}(G, x, y), \{\!\!\{(WL_{2}^{i-1}(G, x, z), WL_{2}^{i-1}(G, z, y))\}\!\!\}_{z \in V(G)},$$
(1)

where $\{\!\!\}\$ denotes the multiset. In words, 2-WL traces through all extensions of each pair (x, y) to a triangle (x, z, y), classifies each (x, z, y) according to the current colors of its sides (x, z) and (z, y), and assigns a new color to each (x, y) so that any two (x, y) and (x', y') become differently colored if they have differently many extensions of some type.

Let \mathcal{P}^i denote the color partition of $V(G)^2$ after the *i*-th refinement. Since \mathcal{P}^i is finer than or equal to \mathcal{P}^{i-1} , the color partition stabilizes starting from some step $t \leq n^2$, where n = |V(G)|, that is, $\mathcal{P}^{t+1} = \mathcal{P}^t$ and, hence, $\mathcal{P}^i = \mathcal{P}^t$ for all $i \geq t$. The algorithm terminates as soon as the stabilization is reached. We denote the final color of a vertex pair (x, y) by $WL_2(G, x, y)$. The following simple observation plays an important role below.

Remark 2.2. The color partition is stable from the very beginning, that is, $\mathcal{P}^1 = \mathcal{P}^0$ and $WL_2(G, x, y) = WL_2^0(G, x, y)$, whenever G is strongly regular, and only in this case.

The k-dimensional version of the algorithm, k-WL, operates similarly with ktuples of vertices and computes a stable color $WL_k(G, x_1, \ldots, x_k)$ for each k-tuple x_1, \ldots, x_k of vertices of G. This coloring extends to s-tuples $\bar{x} = (x_1, \ldots, x_s)$ for s < k and s = k + 1 as follows. If s < k, we set $WL_k(G, \bar{x}) = WL_k(G, x_1, \ldots, x_s, \ldots, x_s)$, i.e., extend \bar{x} to a k-tuple by cloning the last entry. For $\bar{x} = (x_1, \ldots, x_k, x_{k+1})$, we define $WL_k(G, \bar{x}) = (WL_k(G, \bar{x}_{-1}), \ldots, WL_k(G, \bar{x}_{-(k+1)}))$, where \bar{x}_{-i} is obtained from \bar{x} by removing the entry x_i . We do not describe k-WL for $k \geq 3$ in more detail, as the following logical characterization is sufficient for our purposes. Logic with counting quantifiers. Cai, Fürer, and Immerman [6] established a close connection between the Weisfeiler-Leman algorithm and first-order logic with counting quantifiers. A counting quantifier \exists^m opens a logical formula saying that a graph contains at least m vertices with some property. Let C^k denote the set of formulas in the standard first-order logical formalism which can additionally contain counting quantifiers and use occurrences of at most k first-order variables.

Let G be a graph with $s \leq k$ labeled vertices (x_1, \ldots, x_s) . The C^k -type of (G, x_1, \ldots, x_s) is the set of all formulas with s free variables in C^k that are true on (G, x_1, \ldots, x_s) . Despite a rather abstract definition, the C^k -types admit an efficient encoding by the colors produced by the (k-1)-dimensional Weisfeiler-Leman algorithm.

Lemma 2.3 (Cai, Fürer, and Immerman [6]). Let $k \ge 1$ and $0 \le s \le k+1$. Then (G, x_1, \ldots, x_s) and (H, y_1, \ldots, y_s) are of the same C^{k+1} -type if and only if $WL_k(G, x_1, \ldots, x_s) = WL_k(H, y_1, \ldots, y_s)$.

For completeness, we state this result also for k = 1, where 1-WL stands for the classical *degree refinement* routine [15].

3 Local WL invariance

An *s*-labeled graph $F_{\bar{z}}$ is a graph F with a sequence of s (not necessarily distinct) designated vertices $\bar{z} = (z_1, \ldots, z_s)$; cf. [18]. Sometimes we will also use more extensive notation $F_{\bar{z}} = (F, z_1, \ldots, z_s)$, as we already did in Sections 1–2. A homomorphism from an *s*-labeled graph $F_{\bar{z}}$ to an *s*-labeled graph $G_{\bar{x}}$ is a usual homomorphism from F to G taking y_i to x_i for every $i \leq s$.

A tree decomposition of an s-labeled graph $F_{\bar{z}}$ is a tree decomposition of F where there is a bag containing all of the labeled vertices z_1, \ldots, z_s . The treewidth $tw(F_{\bar{z}})$ and the homomorphism-hereditary treewidth $htw(F_{\bar{z}})$ are defined in the same way as for unlabeled graphs. Note that, if $F_{\bar{z}}$ is a graph with s pairwise distinct labeled vertices, then $htw(F_{\bar{z}}) = k$ implies that $s \leq k + 1$.

Remark 3.1. As it easily follows from the definition, for every 1-labeled graph F_{z_1} we have $tw(F_{z_1}) = tw(F)$. Similarly, for a 2-labeled graph F_{z_1,z_2} we have $tw(F_{z_1,z_2}) = tw(F)$ whenever the labeled vertices z_1 and z_2 are adjacent.

For two s-labeled graphs, let $\hom(F_{\bar{z}}, G_{\bar{x}})$ denote the number of homomorphisms from $F_{\bar{z}}$ to $G_{\bar{x}}$. For each pattern graph $F_{\bar{z}}$, the count $\operatorname{sub}(F_{\bar{z}}, G_{\bar{x}})$ is an invariant of a host graph $G_{\bar{x}}$. In general, a function f of a labeled graph is an *invariant* if $f(G_{\bar{x}}) = f(H_{\bar{y}})$ whenever $G_{\bar{x}}$ and $H_{\bar{y}}$ are isomorphic (note that an isomorphism, like any homomorphism, must respect the labeled vertices). We say that an invariant f_1 is *determined* by an invariant f_2 if $f_2(G_{\bar{x}}) = f_2(H_{\bar{y}})$ implies $f_1(G_{\bar{x}}) = f_1(H_{\bar{y}})$.

Lemma 3.2 (Dvořák [10, Lemma 4]). For each s-labeled graph $F_{\bar{z}}$, the homomorphism count hom $(F_{\bar{z}}, G_{\bar{x}})$ is determined by the C^{k+1} -type of (G, \bar{x}) , where $k = tw(F_{\bar{z}})$.

Given a pattern graph $F_{\bar{z}}$ with s pairwise distinct labeled vertices $\bar{z} = (z_1, \ldots, z_s)$ and a host graph $G_{\bar{x}}$ with s pairwise distinct labeled vertices $\bar{x} = (x_1, \ldots, x_s)$, let $\operatorname{sub}(F_{\bar{z}}, G_{\bar{x}})$ denote the number of subgraphs S of G with $x_1, \ldots, x_s \in V(S)$ such that there is an isomorphism from F to S mapping z_i to x_i for all $i \leq s$. Using the well-known inductive approach due to Lovász [16] to relate homomorphism and subgraph counts, from Lemma 3.2 we derive a related fact about local invariance of subgraph counts.

Lemma 3.3. For each s-labeled pattern graph $F_{\bar{z}}$, the subgraph count $\operatorname{sub}(F_{\bar{z}}, G_{\bar{x}})$ is determined by the C^{k+1} -type of (G, \bar{x}) , where $k = htw(F_{\bar{y}})$.

Proof. Let hom^{*}($F_{\bar{z}}, G_{\bar{x}}$) denote the number of *injective* homomorphisms from $F_{\bar{z}}$ to $G_{\bar{x}}$. Counting injective homomorphisms and subgraphs is essentially equivalent, since

$$\operatorname{sub}(F_{\bar{z}}, G_{\bar{x}}) = \frac{\operatorname{hom}^*(F_{\bar{z}}, G_{\bar{x}})}{|\operatorname{Aut}(F_{\bar{z}})|},$$

where $\operatorname{Aut}(F_{\bar{z}})$ is the automorphism group of $F_{\bar{z}}$ (as any homomorphism, automorphisms have to respect the labeled vertices). Therefore, it is enough to prove that the injective homomorphism count $\operatorname{hom}^*(F_{\bar{z}}, G_{\bar{x}})$ is determined by the C^{k+1} -type of (G, \bar{x}) .

We use induction on the number of vertices in F. The base case, namely $V(F) = \{z_1\}$, is obvious. Suppose that F has at least two vertices.

Call a partition α of V(F) proper if every element of α is an independent set of vertices in F. The partition of V(F) into singletons is called *discrete*. A proper partition α determines the homomorphic image F/α of F where $V(F/\alpha) = \alpha$ and two elements A and B of α are adjacent if between the vertex sets A and B there is at least one edge in F. Let $\bar{z}/\alpha = (A_1, \ldots, A_s)$ where A_i is the element of the partition α containing z_i . The s-labeled graph $F_{\bar{z}}/\alpha$ is defined by $F_{\bar{z}}/\alpha = (F/\alpha)_{\bar{z}/\alpha}$. Note that

$$\hom(F_{\bar{z}}, G_{\bar{x}}) = \hom^*(F_{\bar{z}}, G_{\bar{x}}) + \sum_{\alpha} \hom^*(F_{\bar{z}}/\alpha, G_{\bar{x}})$$

where the sum goes over the non-discrete proper partitions of V(F). Note also that the number of labeled vertices in each $F_{\bar{z}}/\alpha$ stays s, but some of them may become equal to each other. In this case, we have $\hom^*(F_{\bar{z}}/\alpha, G_{\bar{x}}) = 0$, and all such α can be excluded from consideration.

Now, $\operatorname{hom}(F_{\bar{z}}, G_{\bar{x}})$ is determined by the C^{k+1} -type of (G, \bar{x}) by Lemma 3.2 because $tw(F_{\bar{z}}) \leq htw(F_{\bar{z}})$. Each $\operatorname{hom}^*(F_{\bar{z}}/\alpha, G_{\bar{x}})$ is determined by the C^{k+1} -type of (G, \bar{x}) by the inductive assumption. It follows that $\operatorname{hom}^*(F_{\bar{z}}, G_{\bar{x}})$ is also determined.

4 Implicit regularity properties

In what follows, by *s*-path (resp. *s*-cycle) we mean a path graph P_s (resp. a cycle graph C_s) on *s* vertices.

Theorem 4.1.

- **1.** For each $s \leq 7$, the number of s-paths between distinct vertices x and y in a strongly regular graph G depends only on the adjacency of x and y (and on the parameters of G).
- **2.** For each $3 \le s \le 5$, the number of s-cycles containing two distinct vertices x and y of a strongly regular graph G depends only on the adjacency of x and y (and on the parameters of G).

Proof. Let $s \leq 7$. Suppose that the path P_s goes through vertices z_1, \ldots, z_s in this order and, similarly, the cycle C_s is formed by vertices z_1, \ldots, z_s in this cyclic order. For cycles, $htw(C_s, z_1, z_s) = htw(C_s) = 2$, where the first equality is due to Remark 3.1 and the second equality is noticed in Example 2.1. Let h be an edgesurjective homomorphism from a 2-labeled path (P_s, z_1, z_s) . If $h(z_1) = h(z_s)$, then the image of (P_s, z_1, z_s) under h is also a homomorphic image of (C_{s-1}, z_1, z_1) . If $h(z_1) \neq h(z_s)$, then adding an edge between $h(z_1)$ and $h(z_s)$ does not increase the treewidth of the 2-labeled image graph, which can then be seen as a homomorphic image of (C_s, z_1, z_s) . Therefore, $htw(P_s, z_1, z_s) \leq \max(htw(C_s, z_1, z_s), htw(C_{s-1}, z_1))$. This implies $htw(P_s, z_1, z_s) \leq 2$. A straightforward inspection shows also that $htw(C_s, z_1, z_i) = 2$ for all $i \leq s$ if $s \leq 5$. We conclude by Lemma 3.3 that $\operatorname{sub}(P_s, z_1, z_s; G, x, y)$ for $s \leq 7$ and $\operatorname{sub}(C_s, z_1, z_i; G, x, y)$ for $s \leq 5$ are determined by the C^3 -type of (G, x, y) and hence, by Lemma 2.3, by the canonical color $WL_2(G, x, y)$. As noticed in Remark 2.2, the color is determined by the adjacency of x and y.

The next result applies to a larger class of graphs. The concept of an association scheme appeared in statistics (Bose [3]) and, also known as a homogeneous coherent configuration (Higman [14]), plays an important role in algebra and combinatorics [7, Chapter 17]. The standard definition and an overview of many important results in this area can be found in [8, 22]. For our purposes, an association scheme can be seen as a complete directed graph with colored edges such that

- all loops (x, x) form a separate color class,
- if two edges (x, y) and (x', y') are equally colored, then their transposes (y, x) and (y', x') are equally colored too, and
- the coloring is stable under the 2-WL refinement.

Each non-loop color class, seen as an undirected graph, forms a *constituent graph* of the association scheme; this concept first appeared apparently in [13].

A strongly regular graph and its complement can be seen as the two constituent graphs of an association scheme. Moreover, all distance-regular graphs [5] are constituent graphs (in fact, every connected strongly regular graph is distance-regular). **Lemma 4.2.** Let $\alpha : V^2 \to C$ be a coloring defining an association scheme, and G be a constituent graph of this scheme. Then $WL_2(G, x, y) = WL_2(G, x', y')$ whenever $\alpha(x, y) = \alpha(x', y')$.

Proof. Using the induction on i, we will prove that the equality $\alpha(x, y) = \alpha(x', y')$ implies the equality $WL_2^i(G, x, y) = WL_2^i(G, x', y')$ for every i. In the base case of i = 0 this is true by the definition of a constituent graph. Suppose that the claim is true for some i for all $x, y, x', y' \in V$.

To prove the claim for i + 1, fix x, y, x', y' such that $\alpha(x, y) = \alpha(x', y')$. By the induction assumption, $WL_2^i(G, x, y) = WL_2^i(G, x', y')$. For a pair of colors $p \in C^2$, let $T(p) = \{z : (\alpha(x, z), \alpha(z, y)) = p\}$ and $T'(p) = \{z' : (\alpha(x', z'), \alpha(z', y')) = p\}$. Since α defines an association scheme, this coloring is not refinable by 2-WL. This means that

$$|T(p)| = |T'(p)| \text{ for every } p \in C^2.$$
(2)

By the induction assumption, for every $z \in T(p)$ and $z' \in T'(p)$ we have

$$(\mathrm{WL}_{2}^{i}(G, x, z), \mathrm{WL}_{2}^{i}(G, z, y)) = (\mathrm{WL}_{2}^{i}(G, x', z'), \mathrm{WL}_{2}^{i}(G, z', y')).$$

Along with Equality (2), this implies that

$$\left\{\!\!\left\{\left(\mathrm{WL}_{2}^{i}(G, x, z), \mathrm{WL}_{2}^{i}(G, z, y)\right)\right\}\!\!\right\}_{z \in V} = \left\{\!\!\left\{\left(\mathrm{WL}_{2}^{i}(G, x', z'), \mathrm{WL}_{2}^{i}(G, z', y')\right)\right\}\!\!\right\}_{z' \in V}$$

and, therefore, $\operatorname{WL}_{2}^{i+1}(G, x, y) = \operatorname{WL}_{2}^{i+1}(G, x', y')$, as desired.

Theorem 4.3. Let G be a constituent graph of an association scheme. If $3 \le s \le 7$, then the number of s-cycles containing an edge xy in G does not depend on the choice of xy.

Proof. As already noted in the proof of Theorem 4.1, $htw(C_s, z_1, z_2) = 2$, where two labeled vertices z_1, z_2 are consecutive in C_s . Like in the proof of Theorem 4.1, we conclude that the count $sub(C_s, z_1, z_2; G, x, y)$ is determined by the canonical color $WL_2(G, x, y)$. Let x'y' be another edge of G. By Lemma 4.2, $WL_2(G, x, y) =$ $WL_2(G, x', y')$ or $WL_2(G, x, y) = WL_2(G, y', x')$. It remains to notice that $sub(C_s, z_1, z_2; G, x', y') =$ $sub(C_s, z_1, z_2; G, y', x')$ just because C_s has an automorphism transposing z_1 and z_2 .

The optimality of Theorems 4.1 and 4.3 is certified by Table 1.

Theorem 4.4 below applies to a yet larger class of graphs. Following [11], we call a graph G WL_{1,2}-regular if WL₂(G, x, x) = WL₂(G, x', x') for every two vertices xand x' of G, that is, 2-WL determines a monochromatic coloring of V(G). Applying Lemma 4.2 in the case y = x and y' = x', we see that any constituent graph of an association scheme is WL_{1,2}-regular. More WL_{1,2}-regular graphs can be obtained by observing that this graph class is closed under taking graph complements and that, if G_1 and G_2 are two WL_{1,2}-regular 2-WL-equivalent graphs, then the disjoint union of G_1 and G_2 is also WL_{1,2}-regular. In terms of the theory of coherent configurations [8], a graph G is WL_{1,2}-regular if and only if the *coherent closure* of G is an association scheme.

$F_{\bar{y}}$	$G_{\bar{x}}$	$\operatorname{sub}(F_{\bar{y}};G_{\bar{x}})$
(P_8, x_1, x_8)	(S, a, a')	2500
(P_8, x_1, x_8)	(S, b, b')	2522
(C_6, x_1, x_3)	(S, a, a')	72
(C_6, x_1, x_3)	(S, b, b')	74
(C_6, x_1, x_4)	(S, a, a')	92
(C_6, x_1, x_4)	(S, b, b')	94
(C_8, x_1, x_2)	(\overline{S}, a, a')	48832
(C_8, x_1, x_2)	(\overline{S}, b, b')	48788

Table 1: S and \overline{S} denote the Shrikhande graph and its complement, respectively; a, a', b, and b' are the four vertices in S shown in Figure 1.

Theorem 4.4.

- **1.** For each $s \leq 7$, the number of s-paths emanating from a vertex x in a WL_{1,2}-regular graph G is the same for every x.
- **2.** For each $3 \le s \le 7$, the number of s-cycles containing a vertex x in a WL_{1,2}-regular graph G is the same for every x.

Proof. Taking into account Remark 3.1 and Example 2.1, we obtain $htw(P_s, z_1) = htw(P_s) \leq 2$ and $htw(C_s, z_1) = htw(C_s) = 2$. Like in the proofs of Theorems 4.1 and 4.3, we conclude that the counts $sub(P_s, z_1; G, x)$ and $sub(C_s, z_1; G, x)$ are determined by the canonical color $WL_2(G, x, x)$. By the definition of $WL_{1,2}$ -regularity, this color is the same for all vertices of G.

Theorem 4.4 is optimal regarding the restriction $s \leq 7$. Indeed, consider the strongly regular graphs with parameters (25, 12, 5, 6) without nontrivial automorphisms. These are two complementary graphs. Specifically, we pick $H = P_{25.02}$ (with graph6 code X}rU\adeSetTjKWNJEYNR]PL jPBgUGVTkK^YKbipMcxbk'{D1XF} in the graph database [4], which is based in this part on [19]. The graph H has a vertex x with sub $(P_8, z_1, H, x) = 11115444$ and sub $(C_8, z_1, H, x) = 5201448$ and a vertex y with sub $(P_8, z_1, H, x) = 11115510$ and sub $(C_8, z_1, H, x) = 5201580$.

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