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SOME REMARKS ON ITERATED LINE GRAPHS ON CAYLEY GRAPHS

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Abstract. This article investigates the properties of iterated line graphs derived from Cayley graphs of finitely generated groups. We study their graph-theoretical properties such as diameter and automorphism groups, and present recursive algorithms for their construction. We show that while these iterated graphs preserve certain algebraic properties, their size grows exponentially and their diameters grow linearly. A generalization of Whitney's theorem about the automorphism groups is presented.

Keywords. Cayley graph, line graph, iterated line graph, group action, computational group theory.
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1. Introduction

In the present article, we study the structural and algorithmic properties of iterated line graphs constructed from Cayley graphs. A Cayley graph $\Gamma(G, S)$ serves as a fundamental combinatorial representation of a finitely generated group G with a generating set S. In general, their spectral properties are known to be closely related to the algebraic and geometric properties of the group and their irreducible characters, see [10, 4, 1]. Beyond the classical Cayley graphs, various generalizations exist, including higher-order iterated line graphs, denoted $\Gamma^K(G, S)$, see [3, 11]. For $K \geq 2$, the vertices of $\Gamma^K(G, S)$ are defined as all possible paths of length $K - 1$ in the underlying Cayley graph $\Gamma(G, S)$, with edges representing successive paths. In general, iterated line graphs are used in the analysis of certain dynamical systems where states and transitions are modeled by vertices and edges of an iterated line graph, see [14].

In this article, we study the graph theoretical properties, such as the diameter and the automorphism group, of iterated line graphs, which are structures that grow exponentially. This type of methodology may have applications involving monads and Kleisli categories in the settings of free categories derived from graphs. We also discuss the algorithmic challenges involved in their construction.

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We present an extension of Whitney's theorem, see [15, 8], to Cayley graphs and their iterated line graphs. Specifically, Theorem 3.5 asserts that for a finitely generated group G and a finite generating set S, the automorphism group of $\Gamma^K(G,S)$ is isomorphic to the automorphism group of $\Gamma(G,S)$ for all $K \geq 2$. A direct consequence of this isomorphism is that the original group G embeds into the automorphism group of $\Gamma^K(G,S)$ for all $K \geq 2$.

Structure of the paper is as follows. In Section 2 we present basic definitions related to Cayley graphs. In Section 3, we focus on structural properties of the Cayley graph $\Gamma^K(G,S)$. In Theorem 3.4, we show that diameter of iterated line graphs grow linearly with respect to that of $\Gamma(G,S)$. In Theorem 3.5, we prove that automorphism groups of a Cayley graph and its iterated line graphs are identical. In Section 4 we focus on algorithmic challenges associated with constructing iterated line graphs. Algorithm 2 introduces the GeneratePaths function, a recursive and divide-and-conquer style component for identifying and enumerating all paths of a specified length K within a given graph $\mathcal{H}$. Algorithm 3 introduces the GraphIteration function which recursively constructs the K-th iterated line graph $\mathcal{H}^K$ from an initial graph $\mathcal{H}$.

2. Notation and Terminology

Following the notations of [14], a (directed) graph $\mathcal{H} = (H^0, H^1, i, t)$ consists of nonempty sets H^0 and H^1 and maps $i, t : H^1 \to H^0$, also see [3]. The elements of H^0 are called vertices and the elements of H^1 are called edges of $\mathcal{H}$. The maps i and t are called initial and terminal maps. We say that the graph $\mathcal{H}$ is finite if both H^0 and H^1 are finite sets. We say that $\mathcal{H}$ is symmetric if there exists a one-to-one map $'\colon H^1 \to H^1$ mapping $e \in H^1$ to $e' \in H^1$ such that $i(e) = t(e')$ and $t(e) = i(e')$ for all $e \in H^1$.

A path of length K for $K \geq 2$ in $\mathcal{H}$ is a sequence $(e^1, e^2, \ldots, e^K)$ where e^k is in H^1 for each $1 \leq k \leq K$ and $t(e^k) = i(e^{k+1})$ for $1 \leq k < K$. We denote by H^K the collection of paths of length $K \geq 2$ in $\mathcal{H}$. We also let $\mathcal{H}^K = (H^{K-1}, H^K, i_K, t_K)$ denote the graph whose vertex set is H^{K-1} and whose edge set is H^K with initial and terminal maps

$$i_K(e^1, e^2, \ldots, e^K) = (e^1, e^2, \ldots, e^{K-1}),$$
$$t_K(e^1, e^2, \ldots, e^K) = (e^2, e^3, \ldots, e^K)$$

for $(e^1, e^2, \ldots, e^K) \in H^K$, respectively. We call $\mathcal{H}^K$ the K-th iterated line graph of $\mathcal{H}$, see [3, 11]. For $K = 2$, $\mathcal{H}^2$ is the classical line graph of $\mathcal{H}$. For $K > 2$, $\mathcal{H}^K$ represents higher iterations of the line graph construction. One can show that if $\mathcal{H}$ is symmetric then $\mathcal{H}^K$ is also symmetric for all $K \geq 2$. Several characterization theorems for line graphs can be found in [3, Sect. 4.5].

Let $\mathcal{H}_1 = (H_1^0, H_1^1, i_1, t_1)$ and $\mathcal{H}_2 = (H_2^0, H_2^1, i_2, t_2)$ be two graphs. A homomorphism $\theta\colon \mathcal{H}_1 \to \mathcal{H}_2$ is a pair $\theta = (\theta^0, \theta^1)$ of maps $\theta^0\colon H_1^0 \to H_2^0$ and $\theta^1\colon H_1^1 \to H_2^1$ such that $\theta^0(i_1(e)) = i_2(\theta^1(e))$ and $t_2(\theta^1(e)) = \theta^0(t_1(e))$ for every $e \in H_1^1$. An endomorphism $\theta = (\theta^0, \theta^1)\colon \mathcal{H} \to \mathcal{H}$ is called an automorphism if θ^0 and θ^1 are bijections. The collection of all automorphisms of $\mathcal{H}$ forms a group, denoted by $\mathrm{Aut}(\mathcal{H})$, under component-wise composition of maps.

Let G be a finitely generated non-trivial group with a finite generating set S. Let X be a nonempty left G-space, a set on which G left acts. The graph of the action $\Gamma(G, S, X)$ consists of the set of vertices X and the set of edges $S \times X$. The initial map $i : S \times X \to X$ is defined by $i(s, x) = x$ for $s \in S, x \in X$; and the terminal map $t : S \times X \to X$ is defined by the left action as $t(s, x) = s \cdot x$ for $s \in S, x \in X$. If the left G-action on X is transitive (meaning for any $x, y \in X$, there exists $g \in G$ such that $g \cdot x = y$), then the graph $\Gamma(G, S, X)$ is connected.

Various methods from graph theory can be used on graphs that are derived from algebraic structures, see [10, 5, 4, 2, 16, 13, 12]. The left Cayley graph $\Gamma(G, S)$ of a group G with respect to a generating set S of G is the graph of the action of G on itself by left multiplication. The vertex set of $\Gamma(G, S)$ is G. For any $g, h \in G$, there is an edge (s, g) from g to h in $\Gamma(G, S)$ if and only if $h = sg$ for some $s \in S$. Therefore, an edge exists from g to h if and only if $hg^{-1} \in S$. The left Cayley graph $\Gamma(G, S)$ is connected, see [16], because for any two vertices $g, h \in G$ there exists a path from g to h. This path is formed by a sequence of multiplications by generators that transform g into h. If the identity element 1 of G is not in S, then there are no self-loops in the Cayley graph, as a self-loop at a vertex g would imply $gg^{-1} = 1 \in S$. If the generating set S is inverse closed in G, that is $S = S^{-1} = \{s^{-1} \colon s \in S\}$, then $\Gamma(G, S)$ is symmetric by considering $' \colon S \times G \to S \times G$ defined by $'(s, g) = (s^{-1}, s \cdot g)$ for all $(s, g) \in S \times G$.

We denote by $\Gamma^K(G, S)$ the K-th iterated line graph of a Cayley graph $\Gamma(G, S)$. Similarly, we denote by $\Gamma^K(G, S, X)$ the K-th iterated line graph of an action graph $\Gamma(G, S, X)$. It follows that $1 \in S$ if and only if $\Gamma^K(G, S)$ has a self-loop at one of its vertices for some $K \geq 2$.

Example 2.1. Elementary group actions can be used to obtain iterated line graphs, see Figure 1. The dihedral group D_{12} of order 12 acts on a regular hexagon. The graph of the action contains six vertices and twelve edges showing the action of the generators on vertices of the hexagon. The line graphs $\Gamma^K(G, S, X)$ for $K \geq 2$ are obtained from the graph of the action. We recall that a vertex cover of $\mathcal{H}$ is a subset of vertices $V \subseteq H^0$ such that for every edge $e \in H^1$ at least one of its endpoints is an element of V.

Example 2.2. Figure 2 shows the Cayley graph $\Gamma(G, S)$ of the dihedral group D_{12} with generating set $S = \{a, b\}$ where $a = (123456)$ and $b = (16)(25)(34)$. The line graph $\Gamma^2(G, S)$ contains 24 vertices and 48 edges. Each vertex of $\Gamma^2(G, S)$ corresponds to an edge of the Cayley graph $\Gamma(G, S)$. Similarly, each edge of $\Gamma^2(G, S)$ corresponds to a path of length two in $\Gamma(G, S)$.

3. Some Structural Properties of $\Gamma^K(G, S)$ for $K \geq 2$

One of the central arguments of [6] is that memory, rather than CPU time, is the limiting resource for constructing large Cayley graphs. This critical memory constraint is further amplified when considering the exponential growth in vertices and edges of $\Gamma^K(G, S)$. This directly supports the next result regarding the exponential growth and memory intensity of the iterated line graphs obtained from Cayley graphs.

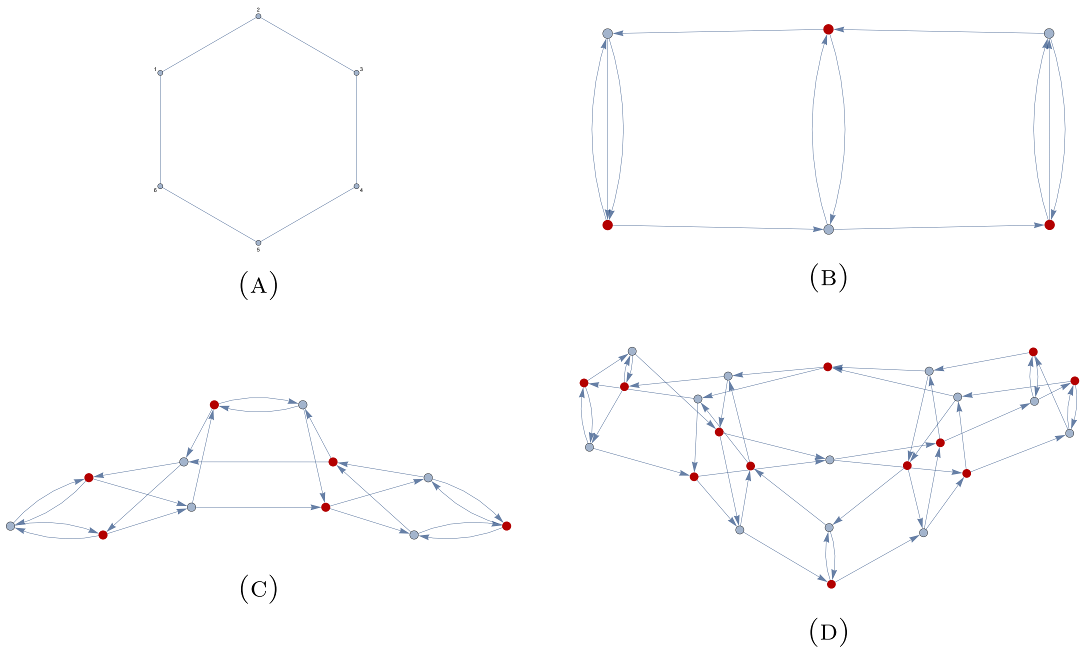

Figure 1. (A) The dihedral group D_{12} generated by $a = (123456)$ and $b = (16)(25)(34)$ acting on vertices X of a hexagon. (B) The corresponding graph (with a highlighted vertex cover) of the action $\Gamma(G, S, X)$ with $S = \{a, b\}$. (C) The line graph $\Gamma^2(G, S, X)$. (D) The line graph $\Gamma^3(G, S, X)$.

Proposition 3.1. *Suppose that G is a finite group of order n and $|S| = m$. Then the number of vertices and edges of $\Gamma^K(G, S)$ for $K \geq 2$ are nm^{K-1} and nm^K, respectively. In particular, the length of a Hamiltonian cycle of $\Gamma^K(G, S)$ is nm^{K-1}.*

Proof. We use induction of K. The vertices of $\Gamma^2(G, S)$ are paths of length one in $\Gamma(G, S)$ and edges of $\Gamma^2(G, S)$ are paths of length two in $\Gamma(G, S)$. As a path of length one of $\Gamma(G, S)$ is nothing but an edge of $\Gamma(G, S)$, the number of paths of length one of $\Gamma(G, S)$ is nm. Every vertex of $\Gamma(G, S)$ has m outgoing edges. For any edge e of $\Gamma(G, S)$ there are m different paths (e^1, e^2) of length two of $\Gamma(G, S)$ such that $e^1 = e$ and $t(e^1) = i(e^2)$. Therefore, the number of edges of $\Gamma^2(G, S)$ is nm^2.

Now, assume for some $K \geq 2$ that the number of vertices of $\Gamma^K(G, S)$ is nm^{K-1} and the number of edges is nm^K. The vertices of $\Gamma^{K+1}(G, S)$ are the edges of $\Gamma^K(G, S)$, so the number of vertices of $\Gamma^{K+1}(G, S)$ is nm^K.

The edges of $\Gamma^{K+1}(G, S)$ are paths of length two in $\Gamma^K(G, S)$. A path of length two in $\Gamma^K(G, S)$ is a sequence of two edges (P_1, P_2) where P_1, P_2 are edges in $\Gamma^K(G, S)$ and $t_K(P_1) = i_K(P_2)$. Let $P_1 = (e^1, \dots, e^K)$ be an edge in $\Gamma^K(G, S)$. The terminal vertex is $t_K(P_1) = (e^2, \dots, e^K)$. The number of edges in $\Gamma^K(G, S)$ starting at this vertex is the number of edges e^{K+1} in $\Gamma(G, S)$ such that $i(e^{K+1}) = t(e^K)$. Since every vertex in $\Gamma(G, S)$ has out-degree m, there are m such edges. Thus, for each edge in $\Gamma^K(G, S)$, there are m possible edges to form a path of

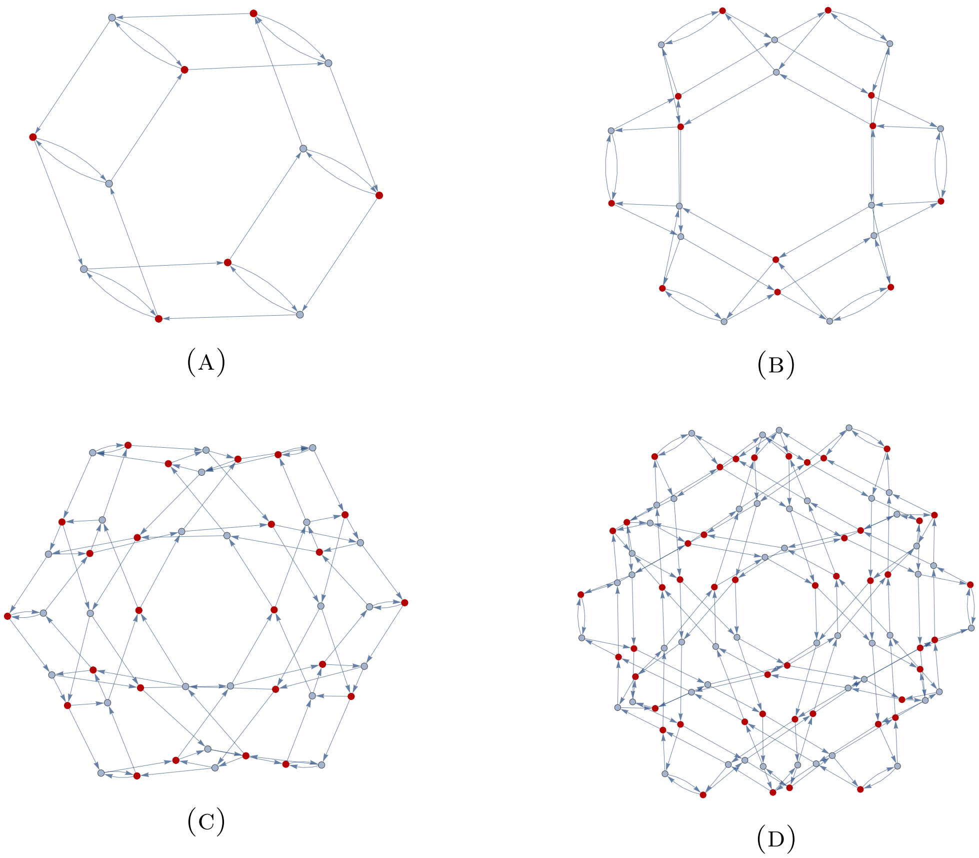

Figure 2. (A) The Cayley Graph $\Gamma(G,S)$ of the dihedral group D_{12} generated by $a=(123456)$ and $b=(16)(25)(34)$ (with a highlighted vertex cover) (B) The graph $\Gamma^2(G,S)$ with $S=\{a,b\}$. (C) The graph $\Gamma^3(G,S)$ with $S=\{a,b\}$. (D) The line graph $\Gamma^4(G,S)$.

length two. Since there are nm^K edges in $\Gamma^K(G,S)$, the total number of edges in $\Gamma^{K+1}(G,S)$ is nm^{K+1}. The result follows by induction. $\square$

Remark 3.2. Let $\mathcal{H}=\Gamma(G,S)$. Denote by H^{K-1} and H^K the vertex and edge sets of $\mathcal{H}^K=\Gamma^K(G,S)$, respectively. A path of length $K-1$ in $\mathcal{H}$ is a sequence $P=(e^1,\ldots,e^{K-1})$ where $e^j=(s_j,g_j)\in H^1$ such that $t(e^j)=i(e^{j+1})$ for $1\le j<K-1$. This implies $s_j\cdot g_j=g_{j+1}$ for $1\le j<K-1$. Such a path is uniquely determined by its starting vertex g_1 and the sequence of generators $(s_1,\ldots,s_{K-1})$. One can represent such a path as $(g_1;s_1,\ldots,s_{K-1})$. Thus, the vertex set of $\mathcal{H}^K$ can be identified with $H^{K-1}=G\times S^{K-1}$ for $K\ge 2$. Similarly, the edge set of $\mathcal{H}^K$ can be identified with $H^K=G\times S^K$. Under these identifications, the initial and terminal maps for $\mathcal{H}^K$ are

$$i_K(g;s_1,\ldots,s_K)=(g;s_1,\ldots,s_{K-1}),$$
$$t_K(g;s_1,\ldots,s_K)=(s_1\cdot g;s_2,\ldots,s_K)$$

for $(g;s_1,\ldots,s_K)\in H^K$, respectively.

The graph density of a nonempty subset V of vertices of a graph $\mathcal{H}$ is the ratio of the number of edges of the induced subgraph of V in $\mathcal{H}$ divided by the number of edges of the complete graph having the same number of vertices as $\mathcal{H}$. The graph density of a graph $\mathcal{H}$ is defined as the graph density of its vertex set. The following result implies that while the number of vertices and edges of $\Gamma^K(G,S)$ grow exponentially with K (making them increasingly large and memory-intensive, see Proposition 3.1) their relative density diminishes.

Corollary 3.3. *Suppose that G is a finite group of order n, $1 \notin S$ and $|S| = m$. Then the graph density of $\Gamma^K(G,S)$ is $\frac{m}{nm^{K-1}-1}$. In particular, the graph density of $\Gamma^K(G,S)$ tends to zero as $K \to \infty$.*

Proof. A simple directed graph with n vertices and m edges has the graph density $\frac{m}{n(n-1)}$. As $1 \notin S$, the graphs $\Gamma(K,S)$ and $\Gamma^K(G,S)$ are simple for $K \geq 2$ as they do not contain self-loops. From Proposition 3.1, the density of $\Gamma^K(G,S)$ is

$$\frac{nm^K}{nm^{K-1}(nm^{K-1}-1)} = \frac{m}{nm^{K-1}-1}$$

for all $K \geq 2$. The particular case follows by taking limit as K tends to infinity. □

The diameter $\operatorname{diam}(\mathcal{H})$ of a connected graph $\mathcal{H}$ is the greatest path distance between any pair of vertices in the graph, see [3, Sect. 2.1]. In the case of Cayley graphs, the distance between any two elements g and h in the group is equivalent to the length of the shortest group word representing the element $g^{-1}h$ in the generating set S, see [1, 10]. In particular, the diameter of $\Gamma(G,S)$ is the greatest shortest path distance between any two group elements. The diameter depends on the choice of the generating set S.

Theorem 3.4. *Suppose that G is a finite group with a generating set S. Then*

$$diam(\Gamma^K(G,S)) = diam(\Gamma(G,S)) + K - 1$$

for all $K \geq 2$.

Proof. We proceed by induction on $K \geq 2$. Let $\ell = \operatorname{diam}(\Gamma(G,S))$. We first show that $\operatorname{diam}(\Gamma^2(G,S)) \leq \ell + 1$. The distance between any two vertices e_1 and e_2 in $\Gamma^2(G,S)$ is at most $\ell + 1$. To see this, let $g = t(e_1)$ and $h = i(e_2)$ be vertices of $\Gamma(G,S)$. Since $\operatorname{diam}(\Gamma(G,S)) = \ell$, the shortest path from g to h has length at most ℓ. Let this path be $(f_1, f_2, \ldots, f_k)$ where $k \leq \ell$ and f_i is an edge of $\Gamma(G,S)$ for $i = 1, 2, \ldots, k$. The sequence

$$((e_1, f_1), (f_1, f_2), \ldots, (f_{k-1}, f_k), (f_k, e_2))$$

of edges of $\Gamma^2(G,S)$ forms a path in $\Gamma^2(G,S)$ from e_1 to e_2 of length $k+1 \leq \ell+1$ in $\Gamma^2(G,S)$. Therefore, the distance between any two vertices e_1 and e_2 in $\Gamma^2(G,S)$ is at most $\ell + 1$.

We show that $\operatorname{diam}(\Gamma^2(G,S)) \geq \ell+1$. Consider two vertices e and e' in $\Gamma^2(G,S)$ for which

$$i(e) = g, \quad t(e) = g', \quad i(e') = h, \quad t(e') = h',$$

where g' and h are maximally distant in $\Gamma(G,S)$. Such e and e' exist because the Cayley graph $\Gamma(G,S)$ is connected. Let $(f^1,\dots,f^\ell)$ be a shortest path in $\Gamma(G,S)$ with $i(f^1)=g'$ and $t(f^\ell)=h$. The distance between e and e' in $\Gamma^2(G,S)$ is realized by the path

$$((e,f^1),(f^1,f^2),\dots,(f^{\ell-1},f^\ell),(f^\ell,e'))$$

in $\Gamma^2(G,S)$ having length $\ell+1$. Any shorter path from e to e' in $\Gamma^2(G,S)$ would require a shorter connection between g' and h in $\Gamma(G,S)$, contradicting the minimality of $(f^1,\dots,f^\ell)$. Therefore, $\operatorname{diam}(\Gamma^2(G,S))\geq \ell+1$

Assume the result holds for $K=n$, i.e., $\operatorname{diam}(\Gamma^n(G,S))=\ell+n-1$. Let us show that it holds for $K=n+1$. We observe that each vertex $P=(e_1,\dots,e_n)$ in $\Gamma^{n+1}(G,S)$ can be mapped to a pair of vertices in $\Gamma^n(G,S)$ via i_n and t_n in such a way that if we put $i_n(P)=P_{\mathrm{i}}=(e_1,\dots,e_{n-1})$ and $t_n(P)=P_{\mathrm{t}}=(e_2,\dots,e_n)$ then an edge from P to Q in $\Gamma^{n+1}(G,S)$ exists if and only if $P_{\mathrm{t}}=Q_{\mathrm{i}}$, i.e., $(e_2,\dots,e_n)=(e'_1,\dots,e'_{n-1})$. Let P and Q be vertices in $\Gamma^{n+1}(G,S)$ realizing the diameter, where $P=(e_1,\dots,e_n)$, and $Q=(e'_1,\dots,e'_n)$ where $e_1,\dots,e_n$ and $e'_1,\dots,e'_n$ are edges of $\Gamma(G,S)$. The distance between P and Q is the length of the shortest path connecting them in $\Gamma^{n+1}(G,S)$. Since $\operatorname{diam}(\Gamma^n(G,S))=\ell+n-1$, the shortest path in $\Gamma^n(G,S)$ connecting P_{t} to Q_{i} has length at most $\ell+n-1$. This path produces a path in $\Gamma^{n+1}(G,S)$ of length at most $\ell+n$ connecting P to Q. This shows that $\operatorname{diam}(\Gamma^{n+1}(G,S))\leq \ell+n$. Conversely, let P and Q be vertices of $\Gamma^{n+1}(G,S)$ such that P_{t} and Q_{i} are maximally distant in $\Gamma^n(G,S)$. The shortest path in $\Gamma^n(G,S)$ connecting P_{t} to Q_{i} has length $\ell+n-1$ by assumption. This path can be lifted to a path from P to Q, namely from $P=(e_1,\dots,e_n)$ the path goes to $(e_2,\dots,e_n,f_1)$ and then $(e_3,\dots,e_n,f_1,f_2)$ and then reaching $(f_{\ell-(n-1)},\dots,f_\ell,e'_1,\dots,e'_{n-1})$ and finally $Q=(e'_1,\dots,e'_n)$ where at each step the edge of $\Gamma^n(G,S)$ appearing in the path becomes a vertex of the path in $\Gamma^n(G,S)$. It follows that the distance between the vertices P and Q in $\Gamma^{n+1}(G,S)$ cannot be less than $\ell+n$. This shows that $\operatorname{diam}(\Gamma^{n+1}(G,S))=\ell+n$. □

By [5, 15f.], automorphism groups of a simple (undirected) graph and its line graph are not always isomorphic. It is a result of H. Whitney, see [15, 9, 8], that for connected simple (undirected) finite graphs having at least 5 vertices, automorphism groups of the graph and its line graph coincide. The only exceptions occur when the graph is K_3 or $K_{1,3}$. A detailed discussion of the exceptional cases can be found in [9]. If a connected graph has 5 or more vertices then every automorphism of its line graph is induced by a unique automorphism of the original graph.

The next result is a generalization of this theorem to the case of directed Cayley graphs. Although the diameter of $\Gamma^K(G,S)$ linearly increases with K, see Theorem 3.4, this does not change the automorphism group.

Theorem 3.5. *Suppose that G is a finitely generated group with a finite generating set $1\notin S$. Then $Aut(\Gamma^K(G,S))$ is isomorphic to $Aut(\Gamma(G,S))$ for all $K\geq 2$. In particular, the group G embeds into $Aut(\Gamma^K(G,S))$ for all $K\geq 2$.*

Proof. Let $\theta=(\theta^0,\theta^1)\in \operatorname{Aut}(\Gamma(G,S))$. For $K\geq 2$, we put $\theta_K(e^1,e^2,\dots,e^K)=(\theta^1(e^1),\theta^1(e^2),\dots,\theta^1(e^K))$ where $(e^1,e^2,\dots,e^K)$ is an edge of $\Gamma^K(G,S)$. We first claim that $\hat{\theta}_K = (\theta_{K-1}, \theta_K)$ with $\theta_1 = \theta^1$ is an automorphism of $\Gamma^K(G,S)$ for $K \geq 2$. Since

$$\theta_{K-1}(i_K(e^1, \ldots, e^K)) = (\theta^1(e^1), \ldots, \theta^1(e^{K-1})) = i_K(\theta_K(e^1, \ldots, e^K))$$

and

$$t_K(\theta_K(e^1, \ldots, e^K)) = (\theta^1(e^2), \ldots, \theta^1(e^K)) = \theta_{K-1}(t_K(e^1, \ldots, e^K))$$

the pair $\hat{\theta}_K = (\theta_{K-1}, \theta_K)$ is an endomorphism of $\Gamma^K(G,S)$. As θ^1 is injective, θ_K is also injective for all $K \geq 2$.

Given $\theta_1 = \theta^1$ is surjective, assume that θ_{K-1} is surjective. Given a path $(e^1, \ldots, e^{K-1}, e^K)$, there exists a path $(f^1, \ldots, f^{K-1})$ such that

$$\theta_{K-1}(f^1, \ldots, f^{K-1}) = (e^1, \ldots, e^{K-1}).$$

As θ^1 is surjective, there exists an edge f^k of $\Gamma(G,S)$ such that $\theta^1(f^K) = e^K$. Since

$$\theta^0(t(f^{K-1})) = t(\theta^1(f^{K-1})) = t(e^{K-1}) = i(e^K) = i(\theta^1(f^K)) = \theta^0(i(f^K))$$

and θ^0 is injective, $t(f^{K-1}) = i(f^K)$, and hence, $(f^1, \ldots, f^{K-1}, f^K)$ forms a path of length K in $\Gamma(G,S)$ satisfying

$$\theta_K(f^1, \ldots, f^{K-1}, f^K) = (e_1, \ldots, e_{K-1}, e_K).$$

Hence, θ_k is surjective.

We claim that the map $\hat{\ }_K \colon \mathrm{Aut}(\Gamma(G,S)) \to \mathrm{Aut}(\Gamma^K(G,S))$ sending $\theta = (\theta^0, \theta^1)$ to $\hat{\theta}_K = (\theta_{K-1}, \theta_K)$ is an injective group homomorphism. Let $\theta = (\theta^0, \theta^1), \gamma = (\gamma^0, \gamma^1) \in \mathrm{Aut}(\Gamma(G,S))$. Then

$$(\hat{\theta\gamma})_K = ((\theta\gamma)_{K-1}, (\theta\gamma)_K) = (\theta_{K-1}\gamma_{K-1}, \theta_K\gamma_K) = \hat{\theta}_K\hat{\gamma}_K,$$

and if θ_K acts as identity on the edge set of $\Gamma^K(G,S)$ then both θ^0 and θ^1 are identities.

To prove surjectivity, we first establish the result for $K = 2$. Then we use the fact that $\Gamma^{K+1}(G,S)$ is the line graph of $\Gamma^K(G,S)$. For showing $\hat{\ }_2 \colon \mathrm{Aut}(\Gamma(G,S)) \to \mathrm{Aut}(\Gamma^2(G,S))$ is surjective, let $(\phi^0, \phi^1) \in \mathrm{Aut}(\Gamma^2(G,S))$. Define $\theta^0(g) = h$ where $h = i(\phi^0(e))$ for some edge e of $\Gamma(G,S)$ satisfying $i(e) = g$. We claim that θ^0 is well defined on vertices of $\Gamma(G,S)$. Let e, e' be two edges of $\Gamma(G,S)$ satisfying $i(e) = i(e') = g$. Denote by P_e the set of vertices f of $\Gamma^2(G,S)$ for which there is an edge from f to e in $\Gamma^2(G,S)$. Because S is finite, the set P_e is finite and nonempty. As $i(e) = i(e')$ one has $P_e = P_{e'}$. Because $\phi^0(P_e) = \phi^0(P_{e'})$, one has $i(\phi^0(e)) = i(\phi^0(e'))$. Hence, $\theta^0(g) = h$ is well defined. We further put $\theta^1 = \phi^0$. We claim that $\theta = (\theta^0, \theta^1) \in \mathrm{Aut}(\Gamma(G,S))$ such that $\hat{\theta}_2 = (\phi^0, \phi^1)$. We have $\theta^0(i(e)) = i(\phi^0(e)) = i(\theta^1(e))$ and $\theta^0(t(e)) = i(\phi^0(f)) = t(\phi^0(e)) = t(\theta^1(e))$ for any f with $e \in P_f$. Let us show that θ^0 is injective. To get a contradiction assume $\theta^0(g_1) = \theta^0(g_2)$ but $g_1 \neq g_2$ for two vertices g_1, g_2 of $\Gamma(G,S)$. Let e_1, e_2 be two edges of $\gamma(G,S)$ with $i(e_1) = g_1$ and $i(e_2) = g_2$ such that $\theta^0(g_1) = i(\phi^0(e_1)) = i(\phi^0(e_2)) = \theta^0(g_2)$. Hence, $P_{\phi^0(e_1)} = P_{\phi^0(e_2)}$. Let $f' \in P_{\phi^0(e_1)}$ and denote by f the unique vertex of $\Gamma^2(G,S)$ such that $\phi^0(f) = f'$. Then $f \in P_{e_1}$ and $f \in P_{e_2}$. This implies that $t(f) = i(e_1) = i(e_2)$, resulting the contradiction $g_1 = g_2$. The map θ^0 is surjective as given vertex h of $\Gamma(G,S)$ there exists an edge e such that

$h = i(\phi^0(e))$ by the surjectivity of ϕ^0. Hence, $\theta^0(i(e)) = h$. Hence $\theta = (\theta^0, \theta^1)$ is indeed an automorphism. Since $(\phi^0, \phi^1) \in \mathrm{Aut}(\Gamma^2(G, S))$, if we put $\phi^1(e_1, e_2) = (e_1', e_2')$ for an edge in $\Gamma^2(G, S)$ then we have $i_2(\phi^1(e_1, e_2)) = \phi^0(i_2(e_1, e_2))$ and $t_2(\phi^1(e_1, e_2)) = \phi^0(t_2(e_1, e_2))$. Hence, $e_1' = \phi^0(e_1)$ and $e_2' = \phi^0(e_2)$. It follows that $\phi^1(e_1, e_2) = (\phi^0(e_1), \phi^0(e_2)) = (\theta^1(e_1), \theta^2(e_2))$. Hence $\hat{\theta}_2 = (\phi^0, \phi^1)$. By the previous discussion, $\mathrm{Aut}(\Gamma(G, S))$ and $\mathrm{Aut}(\Gamma^2(G, S))$ are isomorphic. As $\Gamma^{K+1}(G, S)$ is obtained from $\Gamma^K(G, S)$ in the same way, $\mathrm{Aut}(\Gamma(G, S))$ and $\mathrm{Aut}(\Gamma^K(G, S))$ are isomorphic. In details, for every $K \geq 3$ there is a one to one identification between a path of length two of $\Gamma^{K-1}(G, S)$ to a path of length K of $\Gamma(G, S)$. Up to a labelling of edges, $\Gamma^K(G, S)$ is same as the graph obtained from $\Gamma^{K-1}(G, S)$ by applying the line graph construction.

Consider the right action of G on itself by right multiplication. Every $g \in G$ induces an automorphism $\theta_g = (\theta_g^0, \theta_g^1) \in \mathrm{Aut}(\Gamma(G, S))$ of the left Cayley graph $\Gamma(G, S)$ by defining $\theta_g^0 \colon G \to G$ by $\theta_g^0(h) = hg$ for $h \in G$ and $\theta_g^1 \colon S \times G \to S \times G$ by $\theta_g^1((s, h)) = (s, hg)$ for all $(s, h) \in S \times G$. The map $g \mapsto \theta_g$ is an injective group homomorphism from G into $\mathrm{Aut}(\Gamma(G, S))$. □

Remark 3.6. The embedding of G into $\mathrm{Aut}(\Gamma(G, S))$ appearing in Theorem 3.5 is known to satisfy the property that θ_g^0 is an isometry of $\Gamma(G, S)$ with respect to path distance metric on the vertex set, see [1, 10].

Remark 3.7. In the view of Remark 3.2, let $\theta = (\theta^0, \theta^1)$ be an automorphism of $\Gamma(G, S)$. If $\theta^1(s, g) = (s', g')$ for an edge (s, g) then $i(\theta^1(s, g)) = \theta^0(g)$. Hence, there exists a map $\sigma_g \colon S \to S$ mapping s to s' such that $\theta^1(s, g) = (\sigma_g(s), \theta^0(g))$. The map σ_g is a bijection when S is finite as $\sigma_g(s) = \sigma_g(s')$ for $s, s' \in S$ implies

$$(\sigma_g(s), \theta^0(g)) = \theta^1(s, g) = \theta^1(s', g) = (\sigma_g(s'), \theta^0(g))$$

implies $s = s'$. The automorphism $\hat{\theta}_K = (\theta_{K-1}, \theta_K)$ given in the proof of Theorem 3.5 can be described by

$$\theta_{K-1}(g; s_1, \ldots, s_{K-1}) = (\theta^0(g); \sigma_g(s_1), \sigma_{s_1 \cdot g}(s_2), \ldots, \sigma_{s_{K-2} \cdots s_1 \cdot g}(s_{K-1}))$$

and

$$\theta_K(g; s_1, \ldots, s_K) = (\theta^0(g); \sigma_g(s_1), \sigma_{s_1 \cdot g}(s_2), \ldots, \sigma_{s_{K-1} \cdots s_1 \cdot g}(s_K))$$

4. Algorithmic Construction of $\Gamma^K(G, S)$ for $K \geq 2$

The pseudo-code given in Algorithm 1 is for defining a graph structure, taking sets of vertices and edges as input and returning a formal graph definition, as given in Section 2, that includes initial and terminal maps for its edges. GraphStructure appearing in Algorithm 1 essentially acts as a constructor for an abstract data type representing a directed graph. It takes the vertices and edges and explicitly defines the core operations that give a directed graph its structure, namely, the initial and terminal maps.

In view of Proposition 3.1, memory constraints are a primary bottleneck when constructing Cayley graphs $\Gamma(G, S)$ and their line graphs $\Gamma^K(G, S)$ for $K \geq 2$. This is particularly evident when using memory-intensive graph traversal algorithms like breadth-first search, see [3], to find the shortest paths or spanning

Algorithm 1 Graph Structure Definition Function

1: **Function** GraphStructure(Vertices, Edges)
2: **Input:** Vertices (set H^0), Edges (set H^1)
3: **Output:** A graph structure with initial and terminal maps
4: $i(e) \leftarrow$ Initial vertex of edge e
5: $t(e) \leftarrow$ Terminal vertex of edge e
6: **Return** Graph definition: $\{(H^0, H^1, i, t)\}$

trees in $\Gamma^K(G, S)$. An application of shortest path algorithms is given in the next remark.

Remark 4.1. In a finitely generated group G with generators $s_1, \dots, s_k$ any element $g \in G$ can be expressed as a product of generators and their inverses, see [1]. The number of group words of length at most n describes the growth of the group and are intrinsically linked to the structure of shortest paths in the Cayley graph. The minimal word problem asks for the shortest sequence of generators that produce a given group element, which is equivalent to finding the shortest path from the identity to that element in the Cayley graph $\Gamma(G, S)$. An analogous problem for $\Gamma^K(G, S)$ would be to find the shortest path between two $(K-1)$-length paths, where each step in the path is a new path of length K. This problem seeks to determine the most efficient way to transform one $(K-1)$-length path into another by sequentially appending new edges to its tail and removing from its head, maintaining the specified length K. This is a memory-intensive problem, see Proposition 3.1, as solving such an analogous shortest path problem becomes computationally challenging and memory-intensive, especially with increasing K.

For a Cayley graph $\Gamma(G, S)$ the space complexity is directly proportional to the order of the group $|G|$, as it needs to store representations for each group element as a vertex, see [6]. The time complexity depends on the size of the generating set $|S|$ and the group order $|G|$, often being proportional to $|S||G|$ when using efficient algorithms. For line graphs $\Gamma^K(G, S)$, the challenge becomes significantly more pronounced. As per Proposition 3.1, the exponential growth in the number of vertices and edges with increasing path length K leads to a rapid escalation in memory requirements.

Algorithm 2 introduces the function GeneratePaths that finds all paths of a specified length K within a given graph $\mathcal{H}$. It is a recursive algorithm, using a divide-and-conquer strategy to determine all paths of length K by building upon solutions for paths of length $K-1$. Alternatively, a non-recursive modified breadth-first search, see [3], can find all paths of a given length K by modifying its queue, allowing it to systematically explore all paths layer by layer until the desired length is reached. In all cases, the central primary limitations are their high computational time and space complexities, which are exponential in K, due to the inherent nature of listing all possible paths.

The recursive structure of Algorithm 2 naturally handles graph connectivity, as the algorithm correctly returns an empty set for length K if no paths of length $K-1$ exist, and implicitly stops extending paths that reach dead ends without

Algorithm 2 Algorithm for Creating Vertices of $\mathcal{H}^K$

```
Function GeneratePaths(H, K)
Input: Graph H, Path length K
Output: Set of paths of length K in H
if K = 1 then
    Return All edges of H as paths of length 1
end if
shorterPaths ← GeneratePaths(H, K − 1)
if shorterPaths is empty then
    Return Empty set
end if
paths ← ∅
for each currentPath in shorterPaths do
    lastEdge ← Last edge of currentPath
    lastTerminal ← t(lastEdge)
    for each edge e in H^1 do
        if i(e) = lastTerminal then
            newPath ← Concatenate currentPath and e
            Add newPath to paths
        end if
    end for
end for
Return paths
```

outgoing edges. It starts by returning all individual edges as paths of length one. For lengths greater than one, it generates shorter paths of length $K-1$ and then extends them by appending any valid edge that starts where the shorter path ends.

The GraphIteration function appearing in Algorithm 3 recursively constructs a sequence of iterated graphs, $\mathcal{H}^K$, for a given graph $\mathcal{H}$ and iteration step K. It defines the vertices of $\mathcal{H}^K$ as the paths of length $K-1$ in the original graph $\mathcal{H}$, and its edges as paths of length K. The initial and terminal maps, see Section 2, for edges in $\mathcal{H}^K$ are defined by taking the prefix and suffix paths of length $K-1$, respectively. The base case for the recursion is $K = 1$, where it returns the original graph $\mathcal{H}$. This algorithm essentially builds higher-order graphs where paths in the original graph become vertices or edges in the iterated graphs.

The GeneratePaths function of Algorithm 2 and subsequently GraphIteration function of Algorithm 3 require storing an exponentially growing number of paths, making them computationally prohibitive for larger K or even moderately sized initial graphs. In essence, while CPU time can be a factor, the sheer volume of data generated by the exponential growth of line graphs, especially those of Cayley graphs, quickly overwhelms available memory. This makes memory the critical limiting resource for practical implementations of these graph constructions.

Algorithm 3 Graph Iteration Algorithm

Function GraphIteration($\mathcal{H}$, K)
Input: Graph $\mathcal{H}$, Iteration step K
Output: Graph $\mathcal{H}^K$ and $\mathcal{H}^{K-1}$
if $K \leq 0$ **then**
    Return Error/Failure
end if
if $K = 1$ **then**
    Return (H^0, H^1, i, t), and (H^0, H^1, i, t)
end if
$(\mathcal{H}^{K-1}, \mathcal{H}^{K-2}) \leftarrow$ GraphIteration$(\mathcal{H}, K-1)$
$GKVertices \leftarrow$ GeneratePaths$(\mathcal{H}, K-1)$
$GKEdges \leftarrow$ GeneratePaths$(\mathcal{H}, K)$
Define initial map $i_K(e^1, \ldots, e^K) = (e^1, \ldots, e^{K-1})$
Define terminal map $t_K(e^1, \ldots, e^K) = (e^2, \ldots, e^K)$
$\mathcal{H}_K \leftarrow$ GraphStructure$(GKVertices, GKEdges, i_K, t_K)$
Return $\mathcal{H}^K$, $\mathcal{H}^{K-1}$

The practical efficiency and overall feasibility of GraphIteration are constrained by its reliance on the GeneratePaths sub-function. Consequently, the algorithm's space complexity is dominated by the potentially exponential storage requirements for the sets of paths, GKVertices and GKEdges.

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