Grammar Reinforcement Learning: path and cycle counting in graphs with a Context-Free Grammar and Transformer approach

Anonymous authors
Paper under double-blind review

Abstract

This paper presents Grammar Reinforcement Learning (GRL), a reinforcement learning algorithm that uses Monte Carlo Tree Search (MCTS) and a transformer architecture that models a Pushdown Automaton (PDA) within a context-free grammar (CFG) framework. Taking as use case the problem of efficiently counting paths and cycles in graphs, a key challenge in network analysis, computer science, biology, and social sciences, GRL discovers new matrix-based formulas for path/cycle counting that improve computational efficiency by factors of two to six w.r.t state-of-the-art approaches. Our contributions include: (i) a framework for generating gramformers that operate within a CFG, (ii) the development of GRL for optimizing formulas within grammatical structures, and (iii) the discovery of novel formulas for graph substructure counting, leading to significant computational improvements.

1 Introduction

Paths and cycles are fundamental structures in graph theory, playing a crucial role in various fields such as network analysis (Wang et al., 2023), chemistry (Ishida et al., 2021), computer science (AbuSalim et al., 2020), biology (Bortner and Meshkat, 2022), and social sciences (Boccaletti et al., 2023). Efficiently counting paths and cycles of varying lengths is essential for understanding graph connectivity and network redundancies, and is the foundation of many graph processing algorithms, including graph learning algorithms such as some recent Graph Neural Networks (GNN) (Bouritsas et al., 2022; Michel et al., 2023). In particular, Bouritsas et al. (2022) demonstrated that incorporating precomputed counts of paths or cycles, either at the node level or the graph level, into the feature representation can significantly enhance the expressive power of GNNs.

This problem of counting paths and cycles has been extensively studied in the literature (Harary and Manvel, 1971; Alon et al., 1997; Jokić and Van Mieghem, 2022). Among existing approaches, matrix-based formulae such as those proposed in Voropaev and Perepechko (2012) (see equation (1) for an example) are known to be the most efficient methods for paths and cycles of lengths up to six and seven, respectively (Giscard et al., 2019). This raises a significant open question: Can a deep learning algorithm discover more efficient formulae for counting paths?

In Fürer (2017) and Arvind et al. (2019), the length limits mentioned above are theoretically explained by examining the relationship between the subgraph counting problem and the kth-order Weisfeiler-Leman test (k-WL). These papers conclude that 3-WL cannot count cycles longer than seven. Concurrently, Geerts (2020) explored the connection between 3-WL and a fragment of the matrix language MATLANG (Brijder et al., 2019), defined by the operations $\mathcal{L}_3 := \{\cdot, \ ^{\mathbf{T}}, \mathrm{diag}, \mathbb{1}, \odot\}$. This paper demonstrates that this fragment, when applied to adjacency matrices, distinguishes the same graph pairs as 3-WL. In order to build a 3-WL GNN, Piquenot et al. (2024) introduced a 3-WL Context-Free Grammar (CFG). We observed that, with minor modifications, this generative framework is capable of producing all the formulae previously identified by Voropaev and Perepechko (2012). Taken together,

these recent works enable to transform the search for a path/cycle counting algorithm into a CFG-constrained language generation problem where the aim is to build efficient path counting formulae.

The use of context-free grammars (CFGs) for search has gained considerable attention in the literature. In robotics, Zhao et al. (2020) demonstrated that CFGs can effectively describe robotic structures, enabling the design and adaptation of robots for diverse tasks to be formulated as a search problem within a CFG. Similarly, in the field of AutoML, the application of CFG-based search has been explored (Klinghoffer et al., 2023; Vázquez et al., 2023). In particular, Vazquez et al. (2022) proposed a grammar specifically designed for an AutoML task, where searching within this grammar enables the discovery of the optimal model for a given task.

Searching for formulae within a CFG corresponds to solving a combinatorial optimization problem of possibly infinite size. In recent years, Deep Reinforcement Learning (DRL) approaches have been proposed to address such problems (Vinyals et al., 2015; Khalil et al., 2017; Silver et al., 2018; Hubert et al., 2021; Darvariu et al., 2024). A recent success of DRL has been the discovery of more efficient matrix multiplication algorithms through a Monte Carlo Tree Search (MCTS)-based approach (Fawzi et al., 2022). MCTS-based RL algorithms typically consist of two phases: an acting phase and a learning phase. During the acting phase, the agent selects actions based on a heuristic that combines MCTS exploration with a deep neural network that predicts both policy and value function to guide the tree search. The network is then updated during the learning phase to reflect search trees from multiple iterations. As the objective is to discover efficient formulae and considering that MCTS aligns with CFG sentence generation process due to its tree-based structure, such a Deep MCTS approach is particularly well-suited to searching formulae within CFGs.

In this paper, we propose Grammar Reinforcement Learning (GRL), a deep MCTS model capable of discovering new efficient formulae for path/cycle counting within a CFG. This particular context raises a new research question: How to approximate a policy and a value function through a deep neural network within a CFG?

To address this question, we propose the Gramformer model, a transformer architecture that models Pushdown Automata (PDA), which are equivalent to CFGs. Gramformer is used to learn the policy and value functions within GRL.

When applied to the path/cycle counting problem, GRL not only recovers the formulae from Voropaev and Perepechko (2012) but also discovers new ones, whose computational efficiency is improved by a factor of two to six.

The key contributions of this paper are as follows: (i) We propose GRL, a generic DRL algorithm designed to explore and search within a given grammar. (ii) We introduce Gramformer a new transformer training pipeline compliant with the CFG/PDA framework. (iii) We propose novel state of the art explicit formulae for path/cycle counting in graphs, leading to substantial improvements in computational efficiency.

The structure of this paper is as follows: Section 2 provides the background about path/cycle counting, CFGs and PDAs, defining essential concepts. Section 3 describes the design of GRL, taking as root a given CFG. Section 4 presents Gramformer, connecting transformers and CFGs. Section 5 discusses the results of GRL on path/cycle counting tasks. Finally, we conclude with a summary of our contributions and suggest avenues for future research.

2 Background

2.1 Path and cycle counting

Path and cycle counting in graphs can be performed at multiple levels: graph, node, and edge. At the **graph level**, all possible paths or cycles of a given length within the graph are counted. At the **node level**, the focus is on counting paths starting at a specific node, as well as cycles that include the node. At the **edge level**, for any non-negative integer l, let P_l represent the l-path matrix where $(P_l)_{i,j}$ is the number of l-length paths connecting

vertex i to vertex j. Additionally, for $l > 2$, let C_l represent the l-cycle matrix where $(C_l)_{i,j}$ indicates the number of l-cycles that include vertex i and its adjacent vertex j.

As mentioned in Section 1, path/cycle counting has been extensively tackled in the literature. In the early 1970s, Harary and Manvel (1971) introduced algorithms for counting cycles up to length five at the graph level. Two decades later, Alon et al. (1997) refined these algorithms, extending cycle counting to lengths of up to seven, and conjectured that these methods can also be adapted to count cycles at the node level. Later Voropaev and Perepechko (2012) established a relationship between the counting of l-cycles at the edge level and the counting of $(l-1)$-paths at the edge level using a simple formula. By deriving explicit formulae for the counting of paths of length up to six at the edge level, they were able to compute the number of cycles of length up to seven. More recently, Jokić and Van Mieghem (2022) rediscovered the formulae for paths of length up to four from Voropaev and Perepechko (2012). In contrast, Giscard et al. (2019) proposed an algorithm capable of counting cycles and paths of arbitrary lengths. However, they acknowledged that their method is slower than those presented by Alon et al. (1997) and Voropaev and Perepechko (2012). Specifically, since the latter algorithms are based on matrix multiplication, they exhibit a computational complexity of $O\left(n^3\right)$, where n is the number of nodes. As noted by Giscard et al. (2019), these matrix-based approaches remain the most efficient known methods for counting paths and cycles of lengths up to six and seven, respectively.

2.2 Context-Free Grammar.

Throughout this paper, we employ standard formal language notation: Γ^* denotes the set of all finite-length strings over the alphabet Γ, and ε represents the empty string. The relevant definitions used in this context are as follows:

Definition 2.1 (Context-Free Grammar)
A Context-Free Grammar (CFG) G is defined as a 4-tuple (V, Σ, R, S), where V is a finite set of variables, Σ is a finite set of terminal symbols, R is a finite set of production rules of the form $V \to (V \cup \Sigma)^*$, and S is the start variable. *Note that R fully characterizes the CFG, following the convention that the start variable is placed on the top left and that the symbol $|$ represents "or".*

Definition 2.2 (Derivation)
Let G be a CFG. For $u, v \in (V \cup \Sigma)^*$, we define $u \implies v$ if u can be transformed into v by applying a single production rule, and $u \overset{*}{\implies} v$ if u can be transformed into v by applying a sequence of production rules from G.

Definition 2.3 (Context-Free Language)
A set B is called a Context-Free Language (CFL) if there exists a CFG G such that $B = L(G) := \{w \mid w \in \Sigma^* \text{ and } S \overset{*}{\implies} w\}$.

The generation process in a CFG involves iteratively replacing variables with one of their corresponding production rules, starting from the start variable, until only terminal symbols remain.

As mentioned in Section 1, it is well known that CFGs are equivalent to PDAs (Schneider, 1968; Caucal, 1995; Baeten et al., 2023; DuSell and Chiang, 2024). Usually, PDA are language acceptor, but by relabelling the input as output of the PDA, the same PDA can be used as language generator. Thus the following subsection is dedicated to defining PDA.

2.3 PushDown Automaton

Definition 2.4 (PushDown Automaton)
A PushDown Automaton (PDA) is defined as a 7-tuple $P = (\mathcal{Q}, \Sigma, \Gamma, \delta, q_0, Z, F)$ where $\mathcal{Q}$ is a finite set of states, Σ is a finite set of symbols called the input alphabet, Γ is a finite set of symbol called the stack alphabet, δ is a finite subset of $\mathcal{Q} \times (\Sigma \cup \{\varepsilon\}) \times \Gamma \to \mathcal{Q} \times \Gamma^*$, the transition fuction, $q_0 \in \mathcal{Q}$ is the start state, $Z \in \Gamma$ is the initial stack symbol, $F \subseteq \mathcal{Q}$ is the set of accepting states.

In the case of PDA corresponding to CFG, the input alphabet Σ corresponds to the terminal symbol alphabet. The stack alphabet Γ consits of $V \cup \Sigma$, which is the union of the set of variables (non-terminal symbols) and the terminal symbols. For such a PDA, there are only two states: q_0, the initial state and, $q_1 \in F$, the accepting state. The initial stack symbol is $Z = S$, where S is the start variable of the CFG. The transition fuction δ consists of two types of transitions:

- **Transcription transitions**: If the top of the stack is a terminal symbol $a \in \Sigma$, the transition is of the form $\delta(q_0, a, a) = \{(q_0, \varepsilon)\}$. This indicates that the system remains in state q_0, outputs the symbol a, and removes a from the stack.
- **Transposition transitions**: If the top of the stack is a variable $\nu \in V$, the transition is of the form $\delta(q_0, \varepsilon, \nu) = \{(q_0, r), r \in V_\nu\}$, where $V_\nu \subset R$ is the subset of rules for ν. This means that the system stays in state q_0, produces no output, and replaces ν with the rule r on the stack.

In the same way that production rules fully defines a CFG, the transition fuction δ completely specifies a PDA. For a PDA constructed from a CFG, the transposition transitions alone are sufficient to define the automaton.

A PDA generates a string by starting in the initial state q_0, with the stack initialized to Z and the generated string s initialized to ε. The PDA then processes the top symbol t of the stack according to the transition fuction δ. If $t \in \Sigma$, a transcription occurs: t is popped from the stack and appended to the output string s. If $t \in V = \Gamma \setminus \Sigma$, a transposition occurs: t is popped from the stack, and some $v \in \{v, (q_0, v) \in \delta(q_0, \varepsilon, t)\}$ is pushed onto the stack. Since $v \in \Gamma^*$, it may consist of multiple symbols, which are pushed onto the stack in reverse order. The process continues until the stack is empty, at which point the PDA transitions to the accepting state q_1, and the generated string s is a member of the language of the corresponding CFG.

3 Generating path/cycle counting formula through GRL

The following subsection presents a specific CFG (see Section 2) designed to address the open problem of path counting.

3.1 From path matrix formulae to the CFG G_3

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ denote an undirected graph, where $\mathcal{V} = [\![1\,, n]\!]$ represents the set of n nodes, and $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ represents the set of edges. We define the adjacency matrix $A \in \{0,1\}^{n \times n}$, that encodes the connectivity of $\mathcal{G}$, the identity matrix $\mathrm{I} \in \{0,1\}^{n \times n}$, and the matrix $\mathrm{J} \in \{0,1\}^{n \times n}$, that is filled with ones except along the diagonal.

In the work of Voropaev and Perepechko (2012), all of the proposed formulae are linear combinations of terms composed of matrix multiplications and Hadamard products (denoted by $\odot$) applied exclusively on the arguments A, I, J. For example, the matrix formula in equation (1) is used to count the number of 3-paths between two nodes in the graph. The formulae for path of length four to six can be found in Appendix D of the supplementary material.

$$P_3 = \mathrm{J} \odot A^3 - (\mathrm{I} \odot A^2)A - A(\mathrm{I} \odot A^2) + A \tag{1}$$

To generate the terms of Voropaev's formulae, we define the CFG G_3 in equation (2).

$$M \to (M \odot M) \mid (MM) \mid A \mid \mathrm{I} \mid \mathrm{J}. \tag{2}$$

Voropaev's formulae are linear combinations of sentences of $L(G_3)$. This ensures that the problem of counting paths of length up to 6 can be addressed through finding linear combinations of sentences of $L(G_3)$.

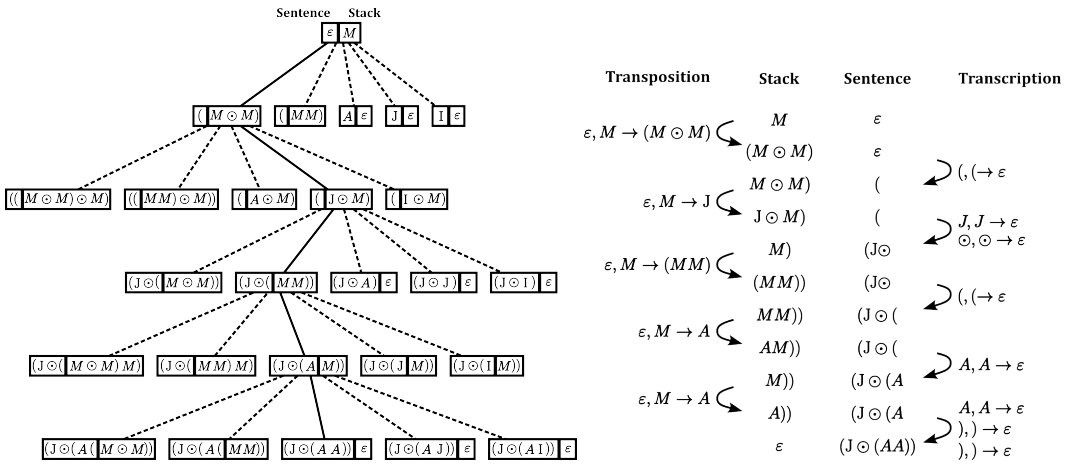


Figure 1: The left diagram illustrates a path in the derivation tree of the PDA D_3 which generates the sentence $J \odot A^2 \in L(G_3)$. The right diagram details the process of generating this sentence, emphasizing the transcription and transposition loops. As depicted, the stack fills during transposition steps and empties during transcription steps, eventually leading to the derivation of a sentence from the language.

Additionally, we prove in Appendix A that G_3 is 3-WL equivalent, resulting in Theorem 3.1.

Theorem 3.1 (3-WL CFG)
G_3 is as expressive as 3-WL

While CFGs are theoretical objects, PDAs are the practical tools for processing and applying the production rules of a CFG to ensure the correct generation of valid sentences according to the grammatical structure. The following subsection derives a PDA (see Section 2) from G_3.

3.2 From G_3 to the PDA D_3

We denote as D_3 the PDA described by the following transition δ:

$$\delta(q_0, \varepsilon, M) = \{(q_0, (M \odot M)), (q_0, (MM)), (q_0, A), (q_0, \mathrm{I}), (q_0, \mathrm{J})\},$$

which corresponds directly to the production rules of G_3.

Figure 1 illustrates how the sentence $(\mathrm{J} \odot (AA)) = J \odot A^2 \in L(G_3)$ is generated by the PDA D_3.

3.3 Search in D_3 through Grammar Reinforcement Learning

To find efficient formulae for path and cycle counting, we propose a two step strategy as illustrated by Figure 2. The first step is to generate a set of sentences belonging to G_3 by the D_3 generation process. The second step compares a linear combination of this set with a ground truth matrix in order to evaluate the corresponding formula. In the following of this subsection, we detail each of these steps.

As stated before, the tree structure of a sentence generation within PDA (see Figure 2) aligns with MCTS algorithm. Such algorithms have been proposed and refined over the last decade to guide the search within trees with a general heuristic (Świechowski et al., 2023). In this work, we propose an MCTS-based DRL algorithm, termed Grammar Reinforcement Learning (GRL) adapted to the path counting open problem, generating sets of different sentences.

In GRL, MCTS performs a series of walks through the PDA, which are stored in a search tree. The nodes of the tree represent states I, which are a concatenation of the written

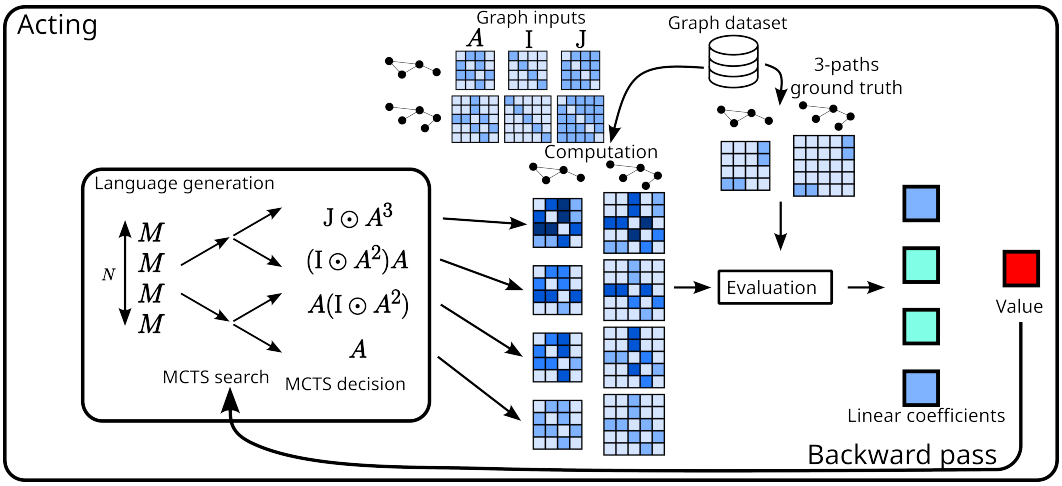


Figure 2: From left to right: The agent selects a set of N sentences based on an MCTS heuristic. These sentences are computed for a given set of graphs. The computation is then evaluated against a ground truth, yielding a linear combination of the sentences and a value representing their pertinence. This value is subsequently backpropagated through the MCTS search tree.

terminal symbols and the stack. The edges correspond to actions defined by the CFG rules r that can be applied at those states.

Each walk begins at the start state $I_0 = \{Z, \cdots, Z\}$, whose cardinality is the number of desired sentences, and terminates when a state contains only terminal symbols. Such terminal states are sets of sentences located in leaf nodes. For each state-action pair (I, r), the algorithm tracks the visit count $N(I, r)$, the empirical rule value $Q(I, r)$, and two scalars predicted by a neural network: a policy probability $\pi(I, r)$ and a value $v(I, r)$. At each intermediate state, a rule action r is selected according to the following equation:

$$\underset{r}{\operatorname{argmax}} \quad \alpha Q(I, r) + (1 - \alpha) v(I, r) + c(I) \pi(I, r) \frac{\sqrt{\sum_a N(I, a)}}{1 + N(I, r)}, \tag{3}$$

where the exploration factor $c(I)$ regulates the influence of the policy $\pi(I, r)$ relative to the Q-values, adjusting this balance based on the frequency of node traversal. The parameter $\alpha \in [0, 1]$ controls the reliance on neural network predictions. After a walk reaches a leaf node, the visit counts and the values are updated via a backward pass.

To update the values, it is necessary to evaluate a leaf node. Its associated set of sentences is computed for a collection of graphs, and a linear combination of these computed sentences is derived by comparing them against a ground truth for each graph. The resulting value, which reflects the relevance of the sentences to a specific path counting problem, is used to empirically update the tree that is constructed during sentence generation. The derivation of this linear combination is detailed in Appendix B, with a specific focus on Figure 8. A concrete example of this approach, applied to the problem of counting 3-paths within G_3, is shown in Figure 2. To encourage the generation of efficient sentences, each CFG rule r is penalized by a value P_r in the reward definition, reflecting its computational cost. Additionally, to prevent the generation of overly long sentences, the number of characters is constrained by a maximum limit, $C_{\max}$.

After a sufficient number of MCTS, the sequences of nodes and edges from each walk are used to train the neural network. The ratio $N(I, r)/N(I)$ provides a policy derived from MCTS exploration, while $Q(I, r)$ represents the empirical expected return for the current state. The policy is learned using a Kullback–Leibler (KL) divergence loss, and the value function is trained using a mean squared error (MSE) loss. The pseudo-code for each algorithm of GRL is provided in Appendix F. Figure 3 depicts both the acting and the learning parts.

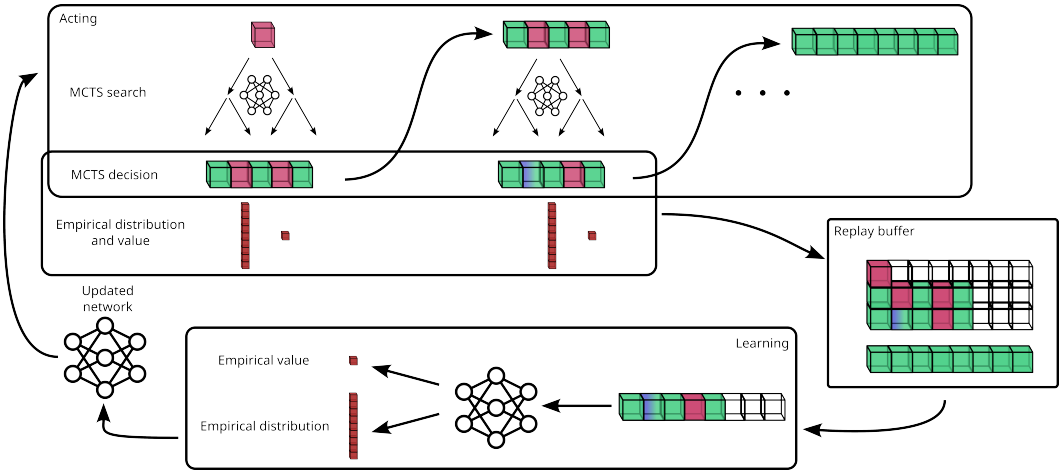


Figure 3: In the acting phase, rules are selected based on both the MCTS algorithm and the neural network outputs. Each time MCTS selects a node, the decision, empirical policy, and value of the node are stored in a replay buffer. During the learning phase, the neural network is updated by predicting the policy and value functions based on the decisions stored in the replay buffer.

The neural network—serving as a memory of the search trees that the agent has previously explored—must be capable of learning the policy and value distributions of the sentence generation within the CFG/PDA. As discussed in Section 1, designing an architecture that can effectively learn within a CFG/PDA remains an open research question. In the next section, we present the neural network used for estimating the policy and value functions in the GRL algorithm.

4 Gramformer

Since our problem is related to the generation of sentences within a language, a transformer architecture fits with this CFG framework. Central to this architecture is the concept of tokens, which represent individual units of input data.

We propose Gramformer, a transformer architecture that follows the production rules of a given CFG, through a PDA. It relies on the assignment of the elements of the transition function δ into three distinct sets of tokens. Recall that δ can be partitioned into two subsets: the transcription set δ_w (for writing) and the transposition set δ_r (for replacing). Specifically, $\delta_r = \{\delta(q_0, \varepsilon, \nu) = \{(q_0, v), v \in R_\nu)\}, \nu \in V\}$, where each $\nu \in V$ represents a variable in the CFG.

For each variable $\nu \in V$, we define a **variable token** corresponding to ν. For each element in $\delta(q_0, \varepsilon, \nu) \in \delta_r$, we define a **rule token** representing the specific production rule. This rule token is divided in two subsets. If the rule contains a variable, the token is classified as a **non-terminal rule token**. If the rule consists only of terminal symbols (i.e., $v \in \Sigma$), the token is classified as a **terminal rule token**. Any symbol in δ_w is assigned as part of the **terminal token** set along with the terminal rule token.

For each variable token, a corresponding mask is provided. This mask indicates the rule tokens associated with that variable. Figure 4 illustrates this framework applied to the CFG G_3 that contains only one variable. An example of a CFG with more variables is provided in Figure 9 of Appendix C. Once all tokens have been defined, the Gramformer is tasked with predicting two ouputs for a given input state. The first output is the probability of selecting the production rule for a given variable. The second one is a scalar that corresponds to the value of the given state.

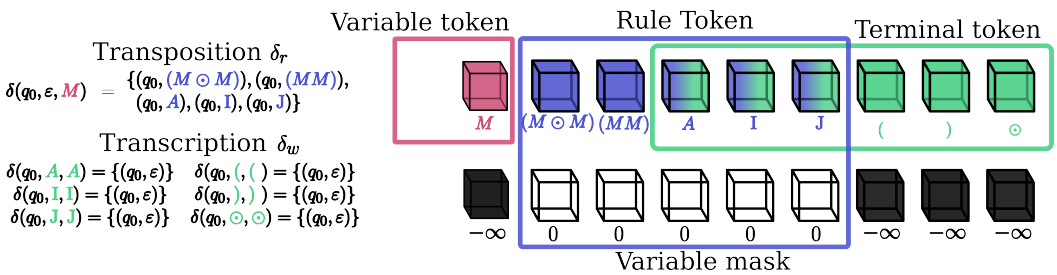


Figure 4: From PDA to grammar tokens: D_3 is turned into three sets of tokens. The corresponding variables of each element of δ_r are turned into variable tokens. For each variable token, a set of rule tokens is defined. Eventually, for every corresponding terminal symbols of δ_w a terminal token is defined. In the end, for each variable token, a variable mask is defined.

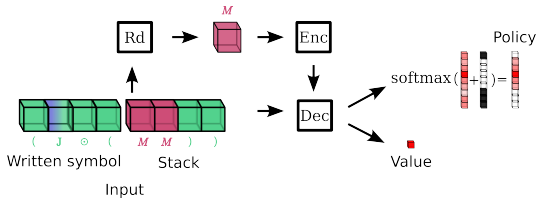


Figure 5: The input is read until the first variable token (**Rd**). This token is passed to the encoder (**Enc**). The decoder (**Dec**) receives the encoder output and the input. The first output of the decoder is combined with the mask corresponding to variable token to generate a policy. The second output is the value.

Gramformer follows a classical encoder-decoder architecture with self-attention and cross-attention mechanisms. At any time, the model's input I consists of the concatenation of the stack and the set of terminal symbols generated so far, representing a state.

The input I is read until a variable token associated to a variable symbol is encountered. This token, denoted as ν is passed to the encoder. The decoder receives the encoder output and the input I. The first output of the decoder is combined with the mask corresponding to ν, so that tokens not associated with ν are set to $-\infty$. This masking ensures that, when the softmax function is applied to the first decoder's output, it yields a valid probability distribution over the rules of ν.

The pseudo-code for each algorithm in this framework is provided in Appendix F. Figure 5 depicts the Gramformer process for a given input.

Note that Gramformer, in an autoregressive mode of operation, can generate sentences within a CFG, simulating a PDA. Figure 6 and Figure 10 of the Appendix C illustrate this generation of the sentence $(\mathrm{J} \odot (AA)) \in L(G_3)$ using the Gramformer architecture coupled with a replace block. The path in the derivation tree of D_3 resulting in the generation of this sentence is provided in Figure 1.

We now have the necessary components to use GRL on the path counting problem, which is described in the following section.

5 Finding more efficient formulae for counting with RL.

To address the problem of path counting at the edge level, we apply GRL using a slightly modified version of the grammar G_3, denoted $\tilde{G}_3$. This grammar generates matrices of $L(G_3)$ with a null diagonal, reducing the search space. For more details on this modified grammar, please refer to Appendix C.

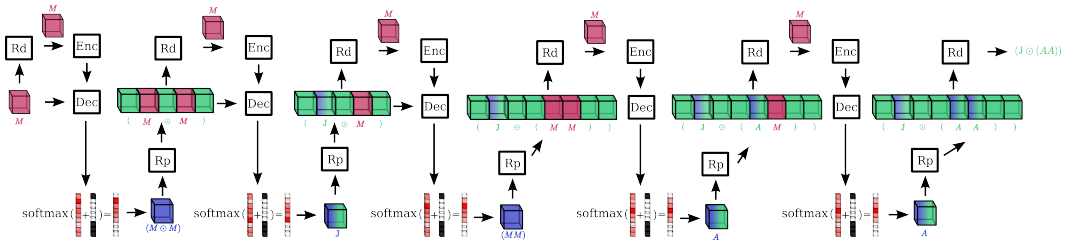


Figure 6: A sequence of tokens is fed into the transformer architecture, beginning with the start variable token. The transformer ouputs the rule token corresponding to the current variable token. The predicted rule's corresponding variables and terminal symbols replace the current variable token, producing a new sequence of tokens. The process is repeated, until no variables remains. At this last step, a sentence from the grammar is generated.

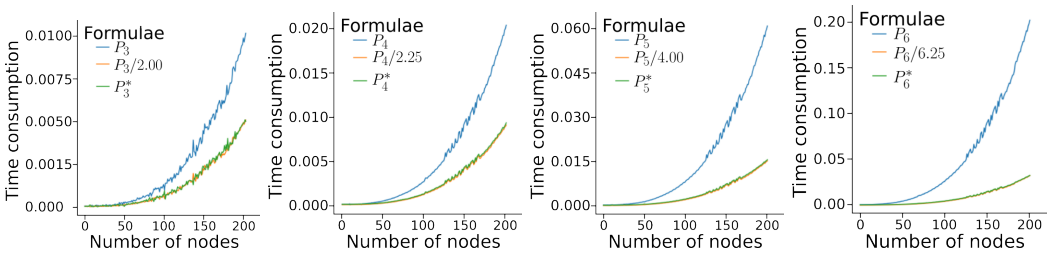


Figure 7: Comparison of the time consumption of P_l and P_l^* in function of the number of nodes for $l \in \{3, 4, 5, 6\}$. Each time, the yellow correspond to the time computation of P_l divided by the theoretical gain of time consumption.

The primary objective of this experiment was to demonstrate that GRL can successfully derive the path counting formulae P_l proposed in Voropaev and Perepechko (2012). Specifically, for $l = 2$, GRL successfully identified the formula P_2. For path lengths $l \in 3, 4, 5, 6$, GRL not only derived the P_l formulae but also discovered more efficient alternatives, denoted as P_l^*. These new formulae significantly reduce the time complexity of l-path counting by factors of 2, 2.25, 4, and 6.25, respectively. The formulae for P_2^* through P_4^* are provided below, while those for P_5^* and P_6^* can be found in Appendix D.

$$
\begin{aligned}
P_2^* &= \mathrm{J} \odot A^2, \\
P_3^* &= \mathrm{J} \odot (A(\mathrm{J} \odot A^2)) - A \odot (A\mathrm{J}), \\
P_4^* &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) - \mathrm{J} \odot (A(A \odot (A\mathrm{J}))) \\
&\quad - \mathrm{J} \odot ((A \odot (A\mathrm{J}))A) - A \odot ((A \odot A^2)\mathrm{J}) + 2A \odot A^2.
\end{aligned}
$$

For each formula, we prove in Appendix D that $P_l = P_l^*$, leading to the following theorem.

Theorem 5.1 (Efficient path counting)
For $l \in \{2, 3, 4, 5, 6\}$, $(P_l^*)_{i,j}$ computes the number of l-paths starting at node i and ending at node j.

It is visually obvious that P_3^* is more compact than P_3. To quantify this, we compare the number of matrix multiplications required, which allows us to derive the ratio of time complexity between the formulae. The theoretical time savings between P_l and P_l^* are detailed in Appendix D.

We also assessed the empirical time savings across various random graphs. For each graph, the time required to compute each formula was recorded, and the average computation time was calculated for graphs of the same size. To compare these results with the theoretical time savings, we divided the mean computation time of P_l by the corresponding theoretical time

reduction factor. The results of these experiments are presented in Figure 7, demonstrating a strong alignment between empirical and theoretical gains. This confirms the significant time savings provided by the new formulae discovered by GRL and supports our theoretical analysis.

In Appendix D, we derive the cycle-counting formulae based on the work of Voropaev and Perepechko (2012), using the relation $C_{l+1} = A \odot P_l$. Additionally, we provide a detailed explanation of how P_l^* counts l-path establishing a new methodology for deriving formulae.

Since 3-WL cannot count the 7-paths (Fürer, 2017), theorem 3.1 leads to the incapability for G_3 to count it either. To go beyond the 6-paths counting, a more expressive grammar is needed.

In Appendix **??**, we evaluate GRL on directed graphs and compare its performance to baseline algorithms. GRL stands out as the only approach capable of discovering novel matrix formulae for counting paths of lengths 4 to 5 in directed graphs.

Resource consumption GRL, like other MCTS based algorithm, suffers from significant resource consumption. For the 5-path and 6-path counting problems, it took weeks to converge. Even with substantial CPU resources (124 AMD EPYC 9654) for the acting and GPU (4 NVIDIA A100) resources for the learning, the process remains extremely time-consuming.

6 Conclusion

This paper introduces Gramformer, a deep learning architecture that learns a policy and a value function within a CFG/PDA framework, by assigning tokens to elements of the transition function of a PDA. Used within the GRL algorithm, it effectively addresses the question "Can a deep learning algorithm discover efficient set of sentences for a given task".

Instantiated over the grammar G_3 to solve the path counting problem, GRL provides efficient formulae that are linear combinations of sets of sentences in $L(G_3)$. These formulae of enhanced computational efficiency by factors ranging from 2 to 6.25 demonstrate the ability of GRL to not only discover explicit formulae for counting paths, but also to provide new ways of designing such formulae.

For paths longer than 6, future research should aim to characterize k-WL CFGs to bypass the theoretical limit on path counting of G_3. Such a characterization will enable the application of GRL to uncover more explicit formulae for substructure counting across graph structures.

Moreover, applying GRL to real-world datasets to derive formulae for various tasks represents a promising direction for future exploration as the grammar provides a link to substructures and thus interpretability.

This approach could potentially improve the applicability and effectiveness of GRL in practical scenarios, thereby broadening its impact.

References

S. W. AbuSalim, R. Ibrahim, M. Z. Saringat, S. Jamel, and J. A. Wahab. Comparative analysis between dijkstra and bellman-ford algorithms in shortest path optimization. In *IOP Conference Series: Materials Science and Engineering*, volume 917, page 012077. IOP Publishing, 2020.

N. Alon, R. Yuster, and U. Zwick. Finding and counting given length cycles. *Algorithmica*, 17(3):209–223, 1997.

V. Arvind, F. Fuhlbrück, J. Köbler, and O. Verbitsky. On weisfeiler-leman invariance: Subgraph counts and related graph properties. In L. A. Gasieniec, J. Jansson, and C. Levcopoulos, editors, *Fundamentals of Computation Theory - 22nd International Symposium, FCT 2019, Copenhagen, Denmark, August 12-14, 2019, Proceedings*, volume 11651 of *Lecture Notes in Computer Science*, pages 111–125. Springer, 2019. doi: 10.1007/978-3-030-25027-0_8. URL `https://doi.org/10.1007/978-3-030-25027-0_8`.

J. C. Baeten, C. Carissimo, and B. Luttik. Pushdown automata and context-free grammars in bisimulation semantics. *Logical Methods in Computer Science*, 19, 2023.

S. Boccaletti, P. De Lellis, C. Del Genio, K. Alfaro-Bittner, R. Criado, S. Jalan, and M. Romance. The structure and dynamics of networks with higher order interactions. *Physics Reports*, 1018:1–64, 2023.

C. Bortner and N. Meshkat. Identifiable paths and cycles in linear compartmental models. *Bulletin of mathematical biology*, 84(5):53, 2022.

G. Bouritsas, F. Frasca, S. Zafeiriou, and M. M. Bronstein. Improving graph neural network expressivity via subgraph isomorphism counting. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 45(1):657–668, 2022.

R. Brijder, F. Geerts, J. V. den Bussche, and T. Weerwag. On the expressive power of query languages for matrices. *ACM Trans. Database Syst.*, 44(4):15:1–15:31, 2019.

D. Caucal. Bisimulation of context-free grammars and of pushdown automata. *Modal Logic and process algebra*, 53:85–106, 1995.

V.-A. Darvariu, S. Hailes, and M. Musolesi. Graph reinforcement learning for combinatorial optimization: A survey and unifying perspective. *arXiv preprint arXiv:2404.06492*, 2024.

B. DuSell and D. Chiang. Stack attention: Improving the ability of transformers to model hierarchical patterns. In *International Conference on Learning Representations*, 2024.

A. Fawzi, M. Balog, A. Huang, T. Hubert, B. Romera-Paredes, M. Barekatain, A. Novikov, F. J. R Ruiz, J. Schrittwieser, G. Swirszcz, et al. Discovering faster matrix multiplication algorithms with reinforcement learning. *Nature*, 610(7930):47–53, 2022.

M. Fürer. On the combinatorial power of the weisfeiler-lehman algorithm. In *International Conference on Algorithms and Complexity*, pages 260–271. Springer, 2017.

F. Geerts. On the expressive power of linear algebra on graphs. *Theory of Computing Systems*, Oct 2020.

P.-L. Giscard, N. Kriege, and R. C. Wilson. A general purpose algorithm for counting simple cycles and simple paths of any length. *Algorithmica*, 81:2716–2737, 2019.

F. Harary and B. Manvel. On the number of cycles in a graph. *Matematickỳ časopis*, 21(1): 55–63, 1971.

T. Hubert, J. Schrittwieser, I. Antonoglou, M. Barekatain, S. Schmitt, and D. Silver. Learning and planning in complex action spaces. In *International Conference on Machine Learning*, pages 4476–4486. PMLR, 2021.

S. Ishida, T. Miyazaki, Y. Sugaya, and S. Omachi. Graph neural networks with multiple feature extraction paths for chemical property estimation. *Molecules*, 26(11):3125, 2021.

I. Jokić and P. Van Mieghem. Number of paths in a graph. *arXiv preprint arXiv:2209.08840*, 2022.

E. Khalil, H. Dai, Y. Zhang, B. Dilkina, and L. Song. Learning combinatorial optimization algorithms over graphs. *Advances in neural information processing systems*, 30, 2017.

T. Klinghoffer, K. Tiwary, N. Behari, B. Agrawalla, and R. Raskar. Diser: Designing imaging systems with reinforcement learning. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 23632–23642, 2023.

G. Michel, G. Nikolentzos, J. F. Lutzeyer, and M. Vazirgiannis. Path neural networks: Expressive and accurate graph neural networks. In *International Conference on Machine Learning*, pages 24737–24755. PMLR, 2023.

J. Piquenot, A. Moscatelli, M. Berar, P. Héroux, R. Raveaux, J.-Y. Ramel, and S. Adam. G^2n^2 : Weisfeiler and lehman go grammatical. In *The Twelfth International Conference on Learning Representations*, 2024.

V. B. Schneider. On the parsing of context-free languages by pushdown automata. In *Ann. meeting of the assoc. for computational linguistics*, number TR-68-76, 1968.

D. Silver, T. Hubert, J. Schrittwieser, I. Antonoglou, M. Lai, A. Guez, M. Lanctot, L. Sifre, D. Kumaran, T. Graepel, et al. A general reinforcement learning algorithm that masters chess, shogi, and go through self-play. *Science*, 362(6419):1140–1144, 2018.

M. Świechowski, K. Godlewski, B. Sawicki, and J. Mańdziuk. Monte carlo tree search: A review of recent modifications and applications. *Artificial Intelligence Review*, 56(3): 2497–2562, 2023.

H. C. Vazquez, J. Sánchez, and R. Carrascosa. Gramml: Exploring context-free grammars with model-free reinforcement learning. In *Sixth Workshop on Meta-Learning at the Conference on Neural Information Processing Systems*, 2022.

H. C. Vázquez, J. Sanchez, and R. Carrascosa. Integrating hyperparameter search into model-free automl with context-free grammars. In *International Conference on Learning and Intelligent Optimization*, pages 523–536. Springer, 2023.

O. Vinyals, M. Fortunato, and N. Jaitly. Pointer networks. *Advances in neural information processing systems*, 28, 2015.

A. Voropaev and S. Perepechko. The number of fixed length cycles in undirected graph explicit formula in case of small lengths. *Discrete and Continuous Models and Applied Computational Science*, (2):6–12, 2012.

J. Wang, W. Liu, L. Chen, X. Li, and Z. Wen. Analysis of china's non-ferrous metals industry's path to peak carbon: A whole life cycle industry chain based on copper. *Science of The Total Environment*, 892:164454, 2023.

A. Zhao, J. Xu, M. Konaković-Luković, J. Hughes, A. Spielberg, D. Rus, and W. Matusik. Robogrammar: graph grammar for terrain-optimized robot design. *ACM Transactions on Graphics (TOG)*, 39(6):1–16, 2020.

This document provides additional content to the main paper.

A CFGs and PDAs

This section provides the proof of theorem 3.1 of Section 2 and more details about PDA.

Even if G_3 is different from the 3-WL CFG proposed in Piquenot et al. (2024), they share the same expressive power. Indeed, in the context of this paper, we are not limited by the depth of the CFG while the goal of the grammar reduction in Piquenot et al. (2024) was to keep the expressiveness of the CFG at a given depth.

It is important to note that in a separative point of view, we separate graphs with scalar, a CFG G separates two graphs $\mathcal{G}_1$ and $\mathcal{G}_2$ if there exists a sentence $s \in L(G)$ such that $s(A_{\mathcal{G}_1}) \neq s(A_{\mathcal{G}_2})$. Knowing that, we have the following proposition and theorem relative to the expressive power of G_3.

Proposition A.1
Assume we have a sentence s that is the sum of two sentences s_1 and s_2. If s separates $\mathcal{G}_1$ and $\mathcal{G}_2$, then it is necessary that s_1 or s_2 separate $\mathcal{G}_1$ and $\mathcal{G}_2$.

Proof. Assume for the sake of contradiction that neither s_1 nor s_2 can separate $\mathcal{G}_1$ and $\mathcal{G}_2$. Then

$$\begin{aligned} s(A_{\mathcal{G}_1}) &= s_1(A_{\mathcal{G}_1}) + s_2(A_{\mathcal{G}_1}) \\ &= s_1(A_{\mathcal{G}_2}) + s_2(A_{\mathcal{G}_2}) = s(A_{\mathcal{G}_2}). \end{aligned}$$

That is absurd. □

Theorem A.1 (3-WL CFG)
G_3 is as expressive as 3-WL

Proof.

$$\begin{aligned} &V_c \to MV_c \mid \mathbb{1} \\ &M \to (M \odot M) \mid (MM) \mid \operatorname{diag}(V_c) \mid A. \end{aligned} \tag{4}$$

We will start from the CFG (4) that was proven to be 3-WL equivalent. We show that V_c variable and $\operatorname{diag}(V_c)$ can be removed.

First of all, we have that for any matrix N and vector w, $Nw = (N \odot \mathrm{I})w + (N \odot \mathrm{J})w$, since a sentence in the CFG (4) consists on a sum other the resulting vector, we have with the help of proposition A.1 that vectors $(N \odot \mathrm{I})w$ and $(N \odot \mathrm{J})w$ have a better separability than Nw. To remove V_c variable, we first have $\mathrm{I} = \operatorname{diag}(\mathbb{1})$. Then for any matrix N and vector w,we have that $(N\operatorname{diag}(w)\,\mathrm{J}) \odot \mathrm{I} = \operatorname{diag}((N \odot \mathrm{J})w)$ and $(N\operatorname{diag}(w)) \odot \mathrm{I} = \operatorname{diag}((N \odot \mathrm{I})w)$.

$$\begin{aligned} (N\operatorname{diag}(w)\,\mathrm{J})_{i,i} &= \sum_{l,m} N_{i,l}\operatorname{diag}(w)_{l,m}\,\mathrm{J}_{m,i} \\ &= \sum_{l} N_{i,l} w_l \mathrm{J}_{l_i} \\ &= \sum_{l} N_{i,l} \mathrm{J}_{i_l} w_l \\ &= \sum_{l} (N \odot \mathrm{J})_{i,l} w_l = ((N \odot \mathrm{J})w)_i, \end{aligned}$$

$$\begin{aligned} (N\operatorname{diag}(w))_{i,i} &= \sum_{l} N_{i,l}\operatorname{diag}(w)_{l,i} \\ &= N_{i,i} w_i \\ &= \sum_{l} (N \odot \mathrm{I})_{i,l} w_l = ((N \odot \mathrm{I})w)_i \end{aligned}$$

The conclusion can be made by induction. We obtain G_3 as expressive as 3-WL. □

To give more insight in the construction of PDA from CFG, consider the PDA D_3, which corresponds to the CFG G_3:

$$D_3 = (\{q_0, q_1\}, \{A, \mathrm{I}, \mathrm{J}, (,), \odot\}, \{M, A, \mathrm{I}, \mathrm{J}, (,), \odot\}, \delta, q_0, M, q_1).$$

where the transition relation δ is defined as follows:

$$\begin{aligned}
&\delta(q_0, \varepsilon, M) = \{(q_0, (M \odot M)), (q_0, (MM)), (q_0, A), (q_0, \mathrm{I}), (q_0, \mathrm{J})\} \\
&\delta(q_0, A, A) = \delta(q_0, \mathrm{I}, \mathrm{I}) = \delta(q_0, \mathrm{J}, \mathrm{J}) = \delta(q_0, (, () = \delta(q_0,),)) = \delta(q_0, \odot, \odot) = \{(q_0, \varepsilon)\} \\
&\delta(q_0, \varepsilon, \varepsilon) = \{(q_1, \varepsilon)\}.
\end{aligned}$$

In the same way that production rules fully defines a CFG, the transition relation δ completely specifies a PDA. For a PDA constructed from a CFG, the transposition transitions alone are sufficient to define the automaton. For instance, D_3 can be fully described by the transition:

$$\delta(q_0, \varepsilon, M) = \{(q_0, (M \odot M)), (q_0, (MM)), (q_0, A), (q_0, \mathrm{I}), (q_0, \mathrm{J})\},$$

which corresponds directly to the production rules of G_3.

B On the evaluation of GRL in the context of path counting

We remind the acting phase of GRL described in section 4. In GRL, an agent generates a set of sentences, $\mathcal{S}$, using a pushdown automaton corresponding to a given CFG. For a given set of graphs, the agent computes the results of each sentence in s. A linear combination of these computed results is then derived and compared to the ground truth path counts, which yields a reward R_s. This section aims to detailed this evaluation process in the case of GRL applied to G_3.

In the case of G_3, the set of computed sentences for a given set of graphs results into a set of matrices for each sentence. We have then s sets of g matrices, where s is the number of sentences and g the number of graphs. Along with this, we have a set of g matrices of ground truth. For the sake of explanation, we assume that each graphs have the same size n. Then we chose s indices $\iota_1, \cdots, \iota_s$ and a graph $\mathcal{G}$ such that, the matrix E of size $s \times s$, where $E_{i,j} = s_j(A_{\mathcal{G}})_{\iota_i}$, is invertible. If such a matrix does not exist, we penalise the set of sentences by attributing a negative value. Along with the construction of E, we define the vector v with the ground truth matrix of $\mathcal{G}$, $T_{\mathcal{G}}$ by $v_i = (T_{\mathcal{G}})_{\iota_i}$.

The linear combination is then obtained by resolving the equation $Ex = v$. Then, the linear combination $\sum_i x_i s_i(A_{\mathcal{G}})$ is compared to the ground truth $T_{\mathcal{G}}$ for all graphs $\mathcal{G}$ resulting in the value $r_{\mathcal{S}}$. This value encompasses the pertinence of the set of sentence $\mathcal{S}$ over a specific path counting problem. Figure 8 depicts this evaluation procedure.

The existence of Voropaev and Perepechko (2012) formulas, ensure that there exist a linear combination of sentences that addresses the path counting of length up to 6.

C A CFG to count at edge level

In our investigation of substructure counting at the edge level for the grammar G_3, we focus on the non-diagonal elements of the involved matrices. To streamline this process, we introduce an alternative context-free grammar, denoted as $\tilde{G}_3$, which is equally expressive as G_3 but specifically tailored for edge-related computations. The grammar is defined as follows:

$$\begin{aligned}
E &\to (E \odot M) \mid (NE) \mid (EN) \mid A \mid \mathrm{J} \\
N &\to (N \odot M) \mid (N \odot N) \mid \mathrm{I} \\
M &\to (MM) \mid (EE)
\end{aligned} \tag{5}$$

In $\tilde{G}_3$, the variable E represents matrices with zero on the diagonal, corresponding to edges in the graph, while N represents diagonal matrices, corresponding to nodes, and M represents

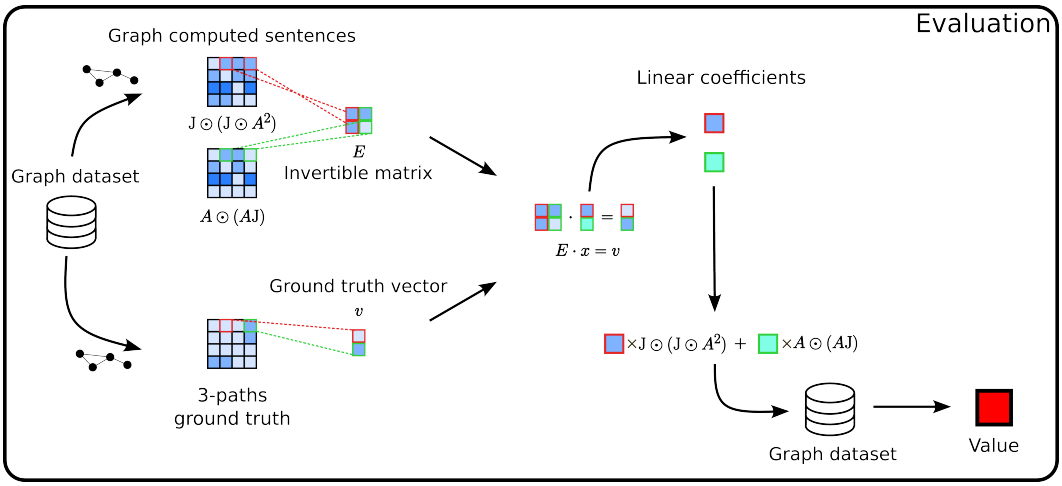


Figure 8: The evaluation process of GRL for path counting involves deriving an invertible matrix E from the computed sentences corresponding to a given graph, alongside a ground truth vector v. The solution of the equation $Ex = v$ provides a linear combination of the computed sentence results. This linear combination is then compared to the ground truth across the entire graph dataset, yielding a value that reflects the effectiveness and relevance of the set of sentences in solving the path counting problem.

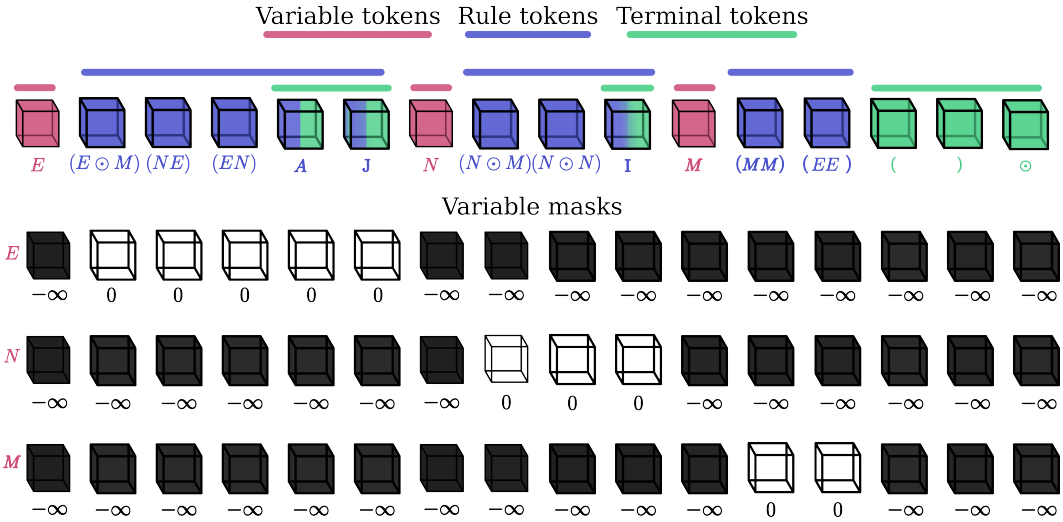


Figure 9: At the top, the tokens of the Graformer derived from $\tilde{G}_3$ are separated into three sets. Below, the variable masks of Gramformer are defined to correspond to the rule tokens of their corresponding variable token.

general matrices. The start variable is E as we aim to focus on edge-level structures. The production rules for each variable describe valid operations and combinations within G_3 that yield matrices corresponding to that variable.

In the case of N, matrix multiplication is omitted because, for diagonal matrices, the matrix product behaves like the Hadamard product. This choice reduces computational complexity without sacrificing expressiveness.

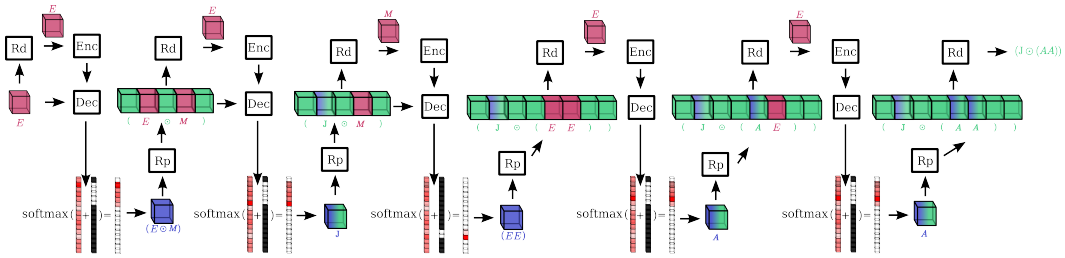


Figure 10: Generation of the sentence $\mathrm{J} \odot A^2 \in L(\tilde{G}_3)$, following a PDA procedure guide by a Gramformer policy.

D Path and cycle counting

This section contains the proof of theorem 5.1 of Section 5 and provides a detailed explanation of how P_l^* counts l-path. In the following, all graphs are assumed to be simple, i.e., they contain no self-loops. This assumption aligns with the search for paths, as self-loops cannot contribute to any path due to the repetition of a node when traversing through a self-loop. Consequently, the adjacency matrix A will always have a zero diagonal. Furthermore, this ensures that $\mathrm{J} \odot A = A$.

As GRL found more efficient formulas to calculate paths and cycles at edge-level in a graph, we tried to prove that such formulas are correct, and by doing so, we found the following lemma that helps to reduce the computation cost.

Lemma D.1
Let N,M and P be square matrices of the same size, such that $N_{i,i} = \sum_k M_{i,k}$ for all indices i. Then we have

$$P \odot (M\mathrm{J}) = (\mathrm{I} \odot N)P - P \odot M$$

Proof. We have

$$\begin{aligned}(P \odot (M\mathrm{J}))_{i,j} &= P_{i,j}(\sum_k M_{i,k} - M_{i,j}) \\ &= P_{i,j}N_{i,i} - P_{i,j}M_{i,j},\end{aligned} \tag{6}$$

and

$$\begin{aligned}((\mathrm{I} \odot N)P - P \odot M)_{i,j} &= \sum_k (\mathrm{I} \odot N)_{i,k}P_{k,j} - P_{i,j}M_{i,j} \\ &= N_{i,i}P_{i,j} - P_{i,j}M_{i,j}.\end{aligned} \tag{7}$$

From equations (6) and (7), we can conclude. □

2-paths and 3-cycles The most effective explicit formula discovered to date for calculating the number of 2-paths connecting two nodes was proposed by Voropaev and Perepechko (2012), it is

$$P_2 = \mathrm{J} \odot A^2. \tag{8}$$

Following the formula for the l-cycle proposed in Voropaev and Perepechko (2012), we obtain for the 3-cycle the following formula

$$C_3 = A \odot P_2 = A \odot A^2. \tag{9}$$

Without any surprise, our architecture found the same formulas for both 2-path and 3-cycle.

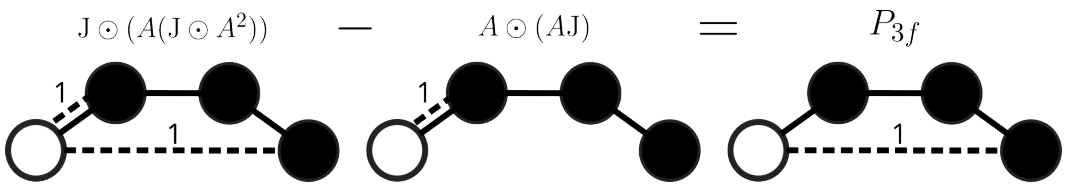


Figure 11: computation of P_3^* for an example graph, the dashed lines indicate an entry in the column corresponding to the white node in the matrix associated with the term specified above.

3-paths and 4-cycles The most effective explicit formula discovered to date for calculating the number of 3-paths connecting two nodes was proposed by Voropaev and Perepechko (2012), it is

$$P_3 = \mathrm{J} \odot A^3 - (\mathrm{I} \odot A^2)A - A(\mathrm{I} \odot A^2) + A. \tag{10}$$

Following the formula for the l-cycle proposed in Voropaev and Perepechko (2012), we obtain for the 3-cycle the following formula

$$C_4 = A \odot P_3 = A \odot A^3 - A(\mathrm{I} \odot A^2) - (\mathrm{I} \odot A^2)A + A. \tag{11}$$

Obviously our architecture found P_3, but surprisingly, it found a more compact formula.

Theorem D.2
The following formula, denoted as P_3^*, computes the number of 3-paths linking two nodes

$$P_3^* = \mathrm{J} \odot (A(\mathrm{J} \odot A^2)) - A \odot (A\mathrm{J}). \tag{12}$$

Proof. We will show that $P_3 = P_3^*$. Firstly, we have

$$\begin{aligned} \mathrm{J} \odot A^3 - A(\mathrm{I} \odot A^2) &= \mathrm{J} \odot ((A(\mathrm{J} + \mathrm{I}) \odot A^2)) - A(\mathrm{I} \odot A^2) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot A^2)) + \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^2))}_{=A(\mathrm{I} \odot A^2)} - A(\mathrm{I} \odot A^2) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot A^2)). \end{aligned} \tag{13}$$

Secondly, we have that $A_{i,i}^2 = \sum_k A_{i,k}$. Thus lemma D.1 implies

$$(\mathrm{I} \odot A^2)A - A = A \odot (A\mathrm{J}). \tag{14}$$

From equality (13) and (14), we can conclude. □

An alternative understanding of how P_3^* computes the number of 3-paths connecting two nodes is illustrated in Figure 11. The process can be described as follows:

The expression $A(\mathrm{J} \odot A^2)$ calculates, from a given node, a non-closed 2-path followed by a 1-path. This computation inherently includes non-closed 3-paths as well as 3-cycles. The 3-cycles are subsequently removed by the Hadamard multiplication with J, which zeroes out the diagonal elements. However, this operation also allows the possibility of traversing a 2-path and then returning to the intermediate node. To account for this and eliminate such paths, we subtract the term $A \odot (A\mathrm{J})$.

Thanks to formula (12), we can derive the 4-cycle formula.

Corollary D.2.1
The following formula, denoted as C_{4f} computes the number of 4-cycles linking two nodes

$$C_{4f} = A \odot (A(\mathrm{J} \odot A^2)) - A \odot (A\mathrm{J}). \tag{15}$$

In terms of time complexity, P_3^* is more efficient than P_3. The ratio of time complexity of P_3^* over P_3 is $\frac{1}{2}$. It is directly derived from the number of matrix multiplications in both formulas. Figure 7 shows the gain of complexity of P_3^* and the ratio between the two formulas.

Surprisingly, even for $l = 3$, GRL allows to improve the computation of path and cycle at edge-level in terms of time complexity.

4-paths and 5-cycles The most effective explicit formula discovered to date for calculating the number of 4-paths connecting two nodes was proposed by Voropaev and Perepechko (2012), it is

$$\begin{aligned} P_4 = \mathrm{J} \odot A^4 - \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) + 2(\mathrm{J} \odot A^2) \\ - (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) \\ - A(\mathrm{I} \odot A^3) - (\mathrm{I} \odot A^3)A + 3A \odot A^2. \end{aligned} \tag{16}$$

Following the formula for the l-cycle proposed in Voropaev and Perepechko (2012), we obtain for the 5-cycle the following formula

$$\begin{aligned} C_5 = A \odot P_4 = A \odot A^4 - A \odot (A(\mathrm{I} \odot A^2)A) \\ - (\mathrm{I} \odot A^2)(A \odot A^2) - (A \odot A^2)(\mathrm{I} \odot A^2) \\ - A(\mathrm{I} \odot A^3) - (\mathrm{I} \odot A^3)A + 5A \odot A^2. \end{aligned} \tag{17}$$

Again, GRL found an improved formula for $l = 4$.

Theorem D.3
The following formula, denoted as P_4^*, computes the number of 4-paths linking two nodes

$$\begin{aligned} P_4^* = \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) - \mathrm{J} \odot (A(A \odot (A\mathrm{J}))) \\ - \mathrm{J} \odot ((A \odot (A\mathrm{J}))A) - A \odot ((A \odot A^2)\mathrm{J}) + 2A \odot A^2. \end{aligned} \tag{18}$$

Proof. We will show that $P_4^* = P_4$. Firstly, we have

$$\begin{aligned} \mathrm{J} \odot A^4 &= \mathrm{J} \odot ((A((\mathrm{J}+\mathrm{I}) \odot A^3))) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot A^3)) + \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^3))}_{=A(\mathrm{I} \odot A^3)} \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^2)))) + A(\mathrm{I} \odot A^3) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) + \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2))))}_{=(\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)} + A(\mathrm{I} \odot A^3) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) + A(\mathrm{I} \odot A^3). \end{aligned} \tag{19}$$

Secondly, we have from equality (14)

$$\begin{aligned} \mathrm{J} \odot ((A \odot (A\mathrm{J}))A) &= \mathrm{J} \odot ((\mathrm{I} \odot A^2)A - A)A) \\ &= \underbrace{\mathrm{J} \odot ((\mathrm{I} \odot A^2)A^2)}_{(\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2)} - \mathrm{J} \odot A^2 \\ &= (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - \mathrm{J} \odot A^2. \end{aligned} \tag{20}$$

Thirdly, we have from equality (14)

$$\begin{aligned} \mathrm{J} \odot (A(A \odot (A\mathrm{J}))) &= \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A - A)) \\ &= \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) - \mathrm{J} \odot A^2. \end{aligned} \tag{21}$$

And eventually, we have $A^3_{i,i} = \sum_k (A \odot A^2)_{i,k}$. Thus lemma D.1 implies

$$(\mathrm{I} \odot A^3)A - A \odot A^2 = A \odot ((A \odot A^2)J). \tag{22}$$

From equality (19), (20),(21) and (22), we can conclude. □

An alternative understanding of how P_4^* computes the number of 4-paths connecting two nodes is illustrated in Figure 12. The process can be described as follows:

The expression $A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2))) - A(A \odot (A\mathrm{J})) = AP_3^*$ calculates, from a given node, a non-closed 3-path followed by a 1-path. This computation inherently includes non-closed 4-paths

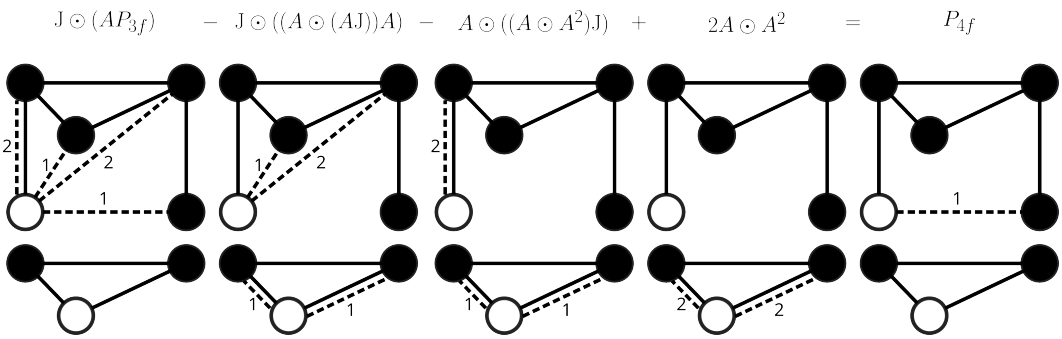


Figure 12: computation of P_4^* for two graphs, the dashed lines indicate an entry in the column corresponding to the white node in the matrix associated with the term specified above.

as well as 4-cycles. The 4-cycles are subsequently removed by the Hadamard multiplication with J, which zeroes out the diagonal elements. However, this operation also allows the possibility of traversing a 3-path and then returning to an intermediate node. To account for this and eliminate respectively paths returning to the third and second nodes of the 3-paths, we subtract the terms $\mathrm{J} \odot ((A \odot (A\mathrm{J}))A) - A \odot A^2$ and $A \odot ((A \odot A^2)\mathrm{J}) - A \odot A^2$.

Thanks to formula (18), we can derive the 5-cycle formula.

Corollary D.3.1
The following formula, denoted as C_{5f} computes the number of 5-cycles linking two nodes

$$\begin{aligned} C_{5f} = {} & A \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) - A \odot (A(A \odot (A\mathrm{J}))) \\ & - A \odot ((A \odot (A\mathrm{J}))A) - A \odot ((A \odot A^2)\mathrm{J}) + 2A \odot A^2. \end{aligned} \tag{23}$$

In terms of time complexity, P_4^* is more efficient than P_4. The ratio of time complexity of P_4^* over P_4 is $\frac{4}{9}$. It is directly derived from the number of matrix multiplications in both formulas. Figure 7 shows the gain of complexity of P_4^* and the ratio between the two formulas.

GRL improves the computation of path and cycle at edge-level for $l = 5$.

5-paths and 6-cycles The most effective explicit formula discovered to date for calculating the number of 5-paths connecting two nodes was proposed by Voropaev and Perepechko (2012), it is

$$\begin{aligned} P_5 = {} & \mathrm{J} \odot A^5 - (\mathrm{I} \odot A^4)A - A(\mathrm{I} \odot A^4) - (\mathrm{I} \odot A^3)(\mathrm{J} \odot A^2) - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^3) \\ & - (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^3) - (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^2) - \mathrm{J} \odot (A(\mathrm{I} \odot A^3)A) + 3A \odot A^3 \\ & + 2A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) + 2(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A + 3A \odot A^2 \odot A^2 + (\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2) \\ & - \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^2) - \mathrm{J} \odot (A^2(\mathrm{I} \odot A^2)A) + 3\mathrm{J} \odot ((A \odot A^2)A) + 3\mathrm{J} \odot (A(A \odot A^2)) \\ & + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A)) - 6(\mathrm{I} \odot A^2)A - 6A(\mathrm{I} \odot A^2) \\ & - 4A \odot A^2 + 3\mathrm{J} \odot A^3 + 4A. \end{aligned} \tag{24}$$

Following the formula for the l-cycle proposed in Voropaev and Perepechko (2012), we obtain for the 6-cycle the following formula

$$\begin{aligned} C_6 = {} & A \odot A^5 - (\mathrm{I} \odot A^4)A - A(\mathrm{I} \odot A^4) - (\mathrm{I} \odot A^3)(A \odot A^2) - (A \odot A^2)(\mathrm{I} \odot A^3) \\ & - (\mathrm{I} \odot A^2)(A \odot A^3) - (A \odot A^3)(\mathrm{I} \odot A^2) - A \odot (A(\mathrm{I} \odot A^3)A) + 6A \odot A^3 \\ & + 2A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) + 2(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A + 3A \odot A^2 \odot A^2 + (\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2) \\ & - A \odot (A(\mathrm{I} \odot A^2)A^2) - A \odot (A^2(\mathrm{I} \odot A^2)A) + 3A \odot ((A \odot A^2)A) + 3A \odot (A(A \odot A^2)) \\ & + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A)) - 6(\mathrm{I} \odot A^2)A - 6A(\mathrm{I} \odot A^2) \\ & - 4A \odot A^2 + 4A. \end{aligned} \tag{25}$$

Again, GRL found an improved formula for $l = 5$.

Theorem D.4
The following formula, denoted as P_5^*, computes the number of 5-paths linking two nodes

$$\begin{aligned} P_5^* &= \mathrm{J} \odot (AP_4^*) - (\mathrm{J} \odot A^2) \odot ((A \odot A^2)\mathrm{J}) - A \odot (C_{4f}\mathrm{J}) - (A\mathrm{J}) \odot P_3^* \\ &\quad + P_3^* + C_{4f} + 2A \odot A^2 \odot A^2 + 3\mathrm{J} \odot ((A \odot A^2)A) - 4A \odot A^2. \end{aligned} \tag{26}$$

Proof. We will show that $P_5^* = P_5$. First, we have

$$\begin{aligned} \mathrm{J} \odot A^5 &= \mathrm{J} \odot ((A((\mathrm{J}+\mathrm{I}) \odot A^4))) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot A^4)) + \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^4))}_{=A(\mathrm{I}\odot A^4)} \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^3)))) + A(\mathrm{I} \odot A^4) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^3)))) + \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^3))))}_{=(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^3)} + A(\mathrm{I} \odot A^4) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^2)))))) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^3) + A(\mathrm{I} \odot A^4) \\ &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))))) + \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)))))) \\ &\quad + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^3) + A(\mathrm{I} \odot A^4). \end{aligned} \tag{27}$$

And

$$\begin{aligned} \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)))))))) &= \mathrm{J} \odot (A(\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)) \\ &= \underbrace{\mathrm{J} \odot (A^3(\mathrm{I} \odot A^2))}_{=(\mathrm{J}\odot A^3)(\mathrm{I}\odot A^2)} - \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2))}_{=A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)} \\ &= (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^2) - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2). \end{aligned} \tag{28}$$

Thus equation (27) and (28) give

$$\begin{aligned} \mathrm{J} \odot A^5 &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))))) + (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^2) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^3) \\ &\quad + A(\mathrm{I} \odot A^4) - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2). \end{aligned} \tag{29}$$

Second, we have from equality (20)

$$\begin{aligned} \mathrm{J} \odot (A(\mathrm{J} \odot ((A \odot (A\mathrm{J}))A))) &= \mathrm{J} \odot (A((\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - \mathrm{J} \odot A^2)) \\ &= \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^2) - \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2))}_{=A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)} - \underbrace{J \odot (A(\mathrm{J} \odot A^2))}_{=\mathrm{J}\odot A^3 - A(\mathrm{I}\odot A^2)} \\ &= \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^2) - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) - \mathrm{J} \odot A^3 \\ &\quad + A(\mathrm{I} \odot A^2). \end{aligned} \tag{30}$$

Third, we have from equality (21)

$$\begin{aligned} \mathrm{J} \odot (A(\mathrm{J} \odot (A(A \odot (A\mathrm{J}))))) &= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) - \mathrm{J} \odot A^2)) \\ &= \mathrm{J} \odot (A^2(\mathrm{I} \odot A^2)A) - \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A)}_{=A(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A)} - \underbrace{J \odot (A(\mathrm{J} \odot A^2))}_{=\mathrm{J}\odot A^3 - A(\mathrm{I}\odot A^2)} \\ &= \mathrm{J} \odot (A^2(\mathrm{I} \odot A^2)A) - A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A) - \mathrm{J} \odot A^3 \\ &\quad + A(\mathrm{I} \odot A^2). \end{aligned} \tag{31}$$

Fourth, we have from equality (22)

$$\begin{aligned} \mathrm{J} \odot (A(A \odot ((A \odot A^2)\mathrm{J}))) &= \mathrm{J} \odot (A((\mathrm{I} \odot A^3)A) - A \odot A^2)) \\ &= \mathrm{J} \odot (A(\mathrm{I} \odot A^3)A) - \mathrm{J} \odot (A(A \odot A^2)). \end{aligned} \tag{32}$$

Fifth, we have $A^3_{i,i} = \sum_k (A \odot A^2)_{i,k}$. Thus lemma D.1 implies

$$(\mathrm{I} \odot A^3)(\mathrm{J} \odot A^2) - A \odot A^2 \odot A^2 = (\mathrm{J} \odot A^2) \odot ((A \odot A^2)J). \tag{33}$$

Sixth, we have $(AP_3^*)_{i,i} = \sum_k (C_{4f})_{i,k}$. Thus lemma D.1 implies

$$(\mathrm{I} \odot (AP_3^*))A - C_{4f} = A \odot (C_{4f}J). \tag{34}$$

Eventually, we have $(A^2)_{i,i} = \sum_k A_{i,k}$. Thus lemma D.1 implies

$$(\mathrm{I} \odot A^2)P_3^* - A \odot P_3^* = P_3^* \odot (A\mathrm{J}). \tag{35}$$

By removing equality (29), (30), (31), (32), (33),(34), (35) and $2J \odot (A(A \odot A^2))$ to P_5, we obtain exactly $P_3^* + C_{4f} + 2A \odot A^2 \odot A^2 + 3\mathrm{J} \odot ((A \odot A^2)A) - 4A \odot A^2$. It concludes the proof. □

An alternative understanding of how P_5^* computes the number of 5-paths connecting two nodes is illustrated in Figure 13. The process can be described as follows:

The expression AP_4^* calculates, from a given node, a non-closed 4-path followed by a 1-path. This computation inherently includes non-closed 5-paths as well as 5-cycles. The 5-cycles are subsequently removed by the Hadamard multiplication with J, which zeroes out the diagonal elements. However, this operation also allows the possibility of traversing a 4-path and then returning to an intermediate node. To account for this and eliminate respectively paths returning to the fourth, third and second nodes of the 4-paths, we subtract the terms $A \odot ((C_{4f})\mathrm{J}) - C_{4f}$, $(\mathrm{J} \odot A^2) \odot ((A \odot A^2)\mathrm{J}) + 4A \odot A^2 - 2A \odot A^2 \odot A^2 - 3\mathrm{J} \odot ((A \odot A^2)A)$ and $(A\mathrm{J}) \odot P_3^* - P_3^*$.

Thanks to formula (26), we can derive the 6-cycle formula.

Corollary D.4.1
The following formula, denoted as C_{6f} computes the number of 6-cycles linking two nodes

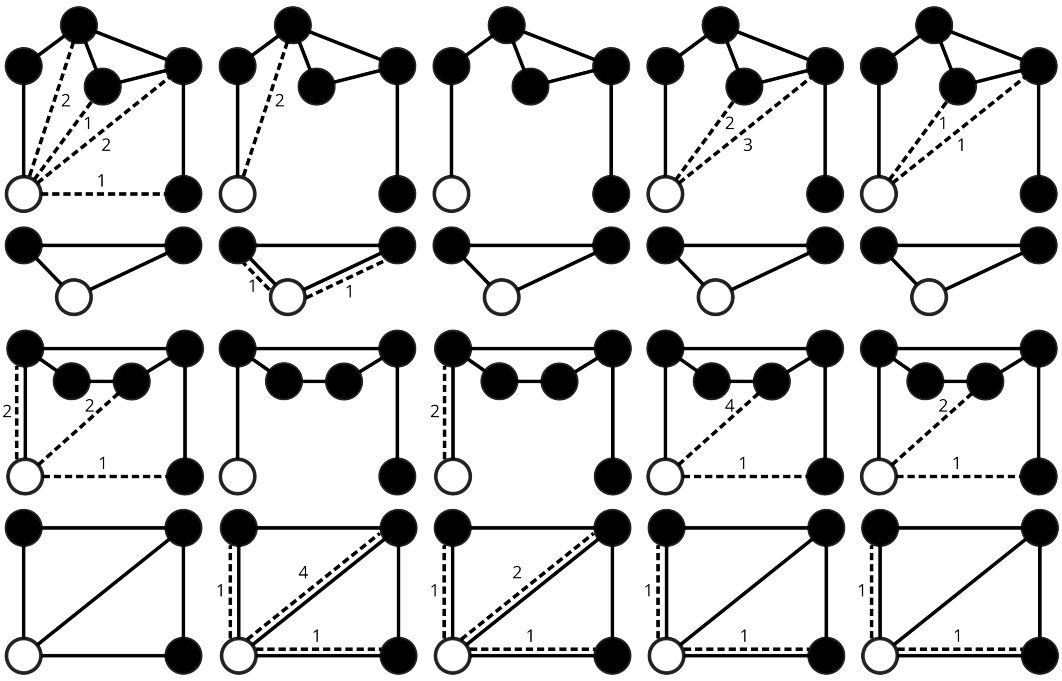
$$\begin{aligned} C_{6f} = {} & A \odot (AP_4^*) - (A \odot A^2) \odot ((A \odot A^2)\mathrm{J}) - A \odot ((C_{4f})\mathrm{J}) - (A\mathrm{J}) \odot C_{4f} \\ & + 2C_{4f} + 2A \odot A^2 \odot A^2 + 3A \odot ((A \odot A^2)A) - 4A \odot A^2. \end{aligned} \tag{36}$$

In terms of time complexity, P_5^* is more efficient than P_5. The ratio of time complexity of P_5^* over P_5 is $\frac{1}{4}$. It is directly derived from the number of matrix multiplications in both formulas. The significant decrease in time complexity can be attributed to the presence of both P_4^*, C_{4f} and P_3^* in the computational formula. The contributions of these terms to the time complexity are cumulative, meaning that each occurrence of P_4^*, C_{4f} and P_3^* adds to the total computational gain. As a result, their individual time complexities are aggregated, leading to the observed diminution in the overall time complexity of the formula. Figure 7 shows the gain of complexity of P_5^* and the ratio between the two formulas.

GRL improves the computation of path and cycle at edge-level for $l = 5$ by a factor 4.

6-paths and 7-cycles The most effective explicit formula discovered to date for calculating the number of 6-paths connecting two nodes was proposed by Voropaev and Perepechko

$$\mathrm{J} \odot (AP_{4f}) - (\mathrm{J} \odot A^2) \odot ((A \odot A^2)\mathrm{J}) - A \odot ((C_{4f})\mathrm{J}) - (A\mathrm{J}) \odot P_{3f} + P_{3f}$$



$$+ C_{4f} - 4A \odot A^2 + 2A \odot A^2 \odot A^2 + 3\mathrm{J} \odot ((A \odot A^2)A) = P_{5f}$$

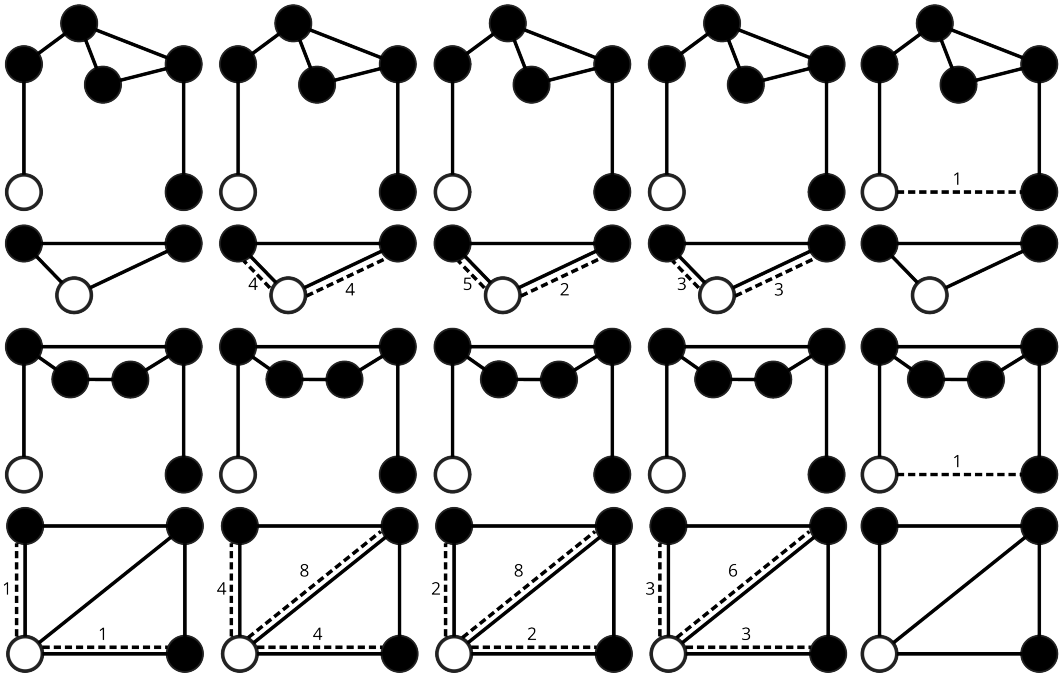


Figure 13: computation of P_5^* for four graphs, the dashed lines indicate an entry in the column corresponding to the white node in the matrix associated with the term specified above.

(2012), it is

$$
\begin{aligned}
P_6 = {} & \mathrm{J} \odot A^6 - (\mathrm{I} \odot A^5)A - A(\mathrm{I} \odot A^5) - (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^4) - (\mathrm{J} \odot A^4)(\mathrm{I} \odot A^2) \\
& - (\mathrm{I} \odot A^4)(\mathrm{J} \odot A^2) - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) - \mathrm{J} \odot (A(\mathrm{I} \odot A^4)A) + 3A \odot A^4 \\
& - (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^3) - (\mathrm{I} \odot A^3)(\mathrm{J} \odot A^3) - \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^3) - \mathrm{J} \odot (A^3(\mathrm{I} \odot A^2)A) \\
& - \mathrm{J} \odot (A(\mathrm{I} \odot A^3)A^2) - \mathrm{J} \odot (A^2(\mathrm{I} \odot A^3)A) + 4A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3) + 4(\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A \\
& + 6A \odot A^2 \odot A^3 + (\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^3) + (\mathrm{I} \odot A^3)A(\mathrm{I} \odot A^2) + 3\mathrm{J} \odot ((A \odot A^3)A) \\
& + 3\mathrm{J} \odot (A(A \odot A^3)) + (\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A)) - \mathrm{J} \odot (A^2(\mathrm{I} \odot A^2)A^2) \\
& + 2A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) + 2(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A + \mathrm{J} \odot A^2 \odot A^2 \odot A^2 + (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) \\
& + 3\mathrm{J} \odot ((A \odot A^2)A^2) + 3\mathrm{J} \odot (A^2(A \odot A^2)) + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))(\mathrm{J} \odot A^2) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A)) \\
& + \mathrm{J} \odot ((\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2)A) + \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2)) + 2\mathrm{J} \odot (A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A) \\
& + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2)) + (\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)A))A + A(\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)A)) \\
& + 3\mathrm{J} \odot ((A \odot A^2 \odot A^2)A) + 3\mathrm{J} \odot (A(A \odot A^2 \odot A^2)) - 12(\mathrm{I} \odot A^2)(A \odot A^2) - 12(A \odot A^2)(\mathrm{I} \odot A^2) \\
& - 4\mathrm{J} \odot A^2 \odot A^2 - 8A \odot (A(A \odot A^2)) - 8A \odot ((A \odot A^2)A) - 3A \odot (A(\mathrm{I} \odot A^2)A) \\
& + 3\mathrm{J} \odot (A(A \odot A^2)A) + \mathrm{J} \odot (A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))A) - 4\mathrm{J} \odot (A(A \odot A^2)) - 4\mathrm{J} \odot ((A \odot A^2)A) \\
& + 4\mathrm{J} \odot A^4 - 5A(\mathrm{I} \odot A^3) - 5(\mathrm{I} \odot A^3)A - 4(\mathrm{I} \odot (A(A \odot A^2)))A - 4A(\mathrm{I} \odot (A(A \odot A^2))) \\
& - 4(\mathrm{I} \odot ((A \odot A^2)A))A - 4A(\mathrm{I} \odot ((A \odot A^2)A)) - 7(\mathrm{I}A^2)(\mathrm{J} \odot A^2) - 7(\mathrm{J} \odot A^2)(\mathrm{I}A^2) \\
& - 10\mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) + 44A \odot A^2 + 12\mathrm{J} \odot A^2.
\end{aligned} \tag{37}
$$

Following the formula for the l-cycle proposed in Voropaev and Perepechko (2012), we obtain for the 7-cycle the following formula

$$
\begin{aligned}
C_7 = {} & A \odot A^6 - (\mathrm{I} \odot A^5)A - A(\mathrm{I} \odot A^5) - (\mathrm{I} \odot A^2)(A \odot A^4) - (A \odot A^4)(\mathrm{I} \odot A^2) \\
& - (\mathrm{I} \odot A^4)(A \odot A^2) - (A \odot A^2)(\mathrm{I} \odot A^4) - A \odot (A(\mathrm{I} \odot A^4)A) + 3A \odot A^4 \\
& - (A \odot A^3)(\mathrm{I} \odot A^3) - (\mathrm{I} \odot A^3)(A \odot A^3) - A \odot (A(\mathrm{I} \odot A^2)A^3) - A \odot (A^3(\mathrm{I} \odot A^2)A) \\
& - A \odot (A(\mathrm{I} \odot A^3)A^2) - A \odot (A^2(\mathrm{I} \odot A^3)A) + 4A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3) + 4(\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A \\
& + 6A \odot A^2 \odot A^3 + (\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^3) + (\mathrm{I} \odot A^3)A(\mathrm{I} \odot A^2) + 3A \odot ((A \odot A^3)A) \\
& + 3A \odot (A(A \odot A^3)) + (\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A)) - A \odot (A^2(\mathrm{I} \odot A^2)A^2) \\
& + 2A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) + 2(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A + A \odot A^2 \odot A^2 \odot A^2 + (\mathrm{I} \odot A^2)(A \odot A^2)(\mathrm{I} \odot A^2) \\
& + 3A \odot ((A \odot A^2)A^2) + 3A \odot (A^2(A \odot A^2)) + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))(A \odot A^2) + (A \odot A^2)(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A)) \\
& + A \odot ((\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2)A) + A \odot (A(\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2)) + 2A \odot (A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)A) \\
& + (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2))A + A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2)) + (\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)A))A + A(\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)A)) \\
& + 3A \odot ((A \odot A^2 \odot A^2)A) + 3A \odot (A(A \odot A^2 \odot A^2)) - 12(\mathrm{I} \odot A^2)(A \odot A^2) - 12(A \odot A^2)(\mathrm{I} \odot A^2) \\
& - 4A \odot A^2 \odot A^2 - 8A \odot (A(A \odot A^2)) - 8A \odot ((A \odot A^2)A) - 3A \odot (A(\mathrm{I} \odot A^2)A) \\
& + 3A \odot (A(A \odot A^2)A) + A \odot (A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))A) - 4A \odot (A(A \odot A^2)) - 4A \odot ((A \odot A^2)A) \\
& + 4A \odot A^4 - 5A(\mathrm{I} \odot A^3) - 5(\mathrm{I} \odot A^3)A - 4(\mathrm{I} \odot (A(A \odot A^2)))A - 4A(\mathrm{I} \odot (A(A \odot A^2))) \\
& - 4(\mathrm{I} \odot ((A \odot A^2)A))A - 4A(\mathrm{I} \odot ((A \odot A^2)A)) - 7(\mathrm{I}A^2)(A \odot A^2) - 7(A \odot A^2)(\mathrm{I}A^2) \\
& - 10A \odot (A(\mathrm{I} \odot A^2)A) + 56A \odot A^2.
\end{aligned} \tag{38}
$$

Again, GRL found an improved formula for $l = 6$.

Theorem D.5
The following formula, denoted as P_6^* computes the number of 6-paths linking two nodes

$$
\begin{aligned}
P_6^* = {} & \mathrm{J} \odot (AP_5^*) - P_3^* \odot ((A \odot A^2)\mathrm{J}) - A \odot (C_{5f}\mathrm{J}) - P_4^* \odot (A\mathrm{J}) \\
& + P_4^* + C_{5f} - (\mathrm{J} \odot A^2) \odot (C_{4f}\mathrm{J}) + 4A \odot A^2 \odot P_3^* + 3\mathrm{J} \odot ((A \odot A^2)(\mathrm{J} \odot A^2)) \\
& + \mathrm{J} \odot A^2 \odot A^2 \odot A^2 + 3\mathrm{J} \odot ((A \odot A^2 \odot A^2)A) - 4\mathrm{J} \odot A^2 \odot A^2 - 8A \odot (A(A \odot A^2)) \\
& - 8A \odot ((A \odot A^2)A) - 4\mathrm{J} \odot ((A \odot A^2)A) - 3A \odot ((A \odot A^2)\mathrm{J}) + 17A \odot A^2 + 3\mathrm{J} \odot A^2.
\end{aligned} \tag{39}
$$

Proof. We will show that $P_6^* = P_6$. First, we have

$$
\begin{aligned}
\mathrm{J} \odot A^6 &= \mathrm{J} \odot ((A((\mathrm{J}+\mathrm{I}) \odot A^5))) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot A^5)) + \underbrace{\mathrm{J} \odot (A(\mathrm{I} \odot A^5))}_{=A(\mathrm{I}\odot A^5)} \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^4)))) + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^4)))) + \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^4))))}_{=(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^4)} + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^3)))))) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^3)))))) + \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^3)))))) }_{=(\mathrm{J}\odot A^3)(\mathrm{I}\odot A^3) - A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^3)} \\
&\qquad + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A((\mathrm{J}+\mathrm{I}) \odot A^2)))))))) + (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^3) \\
&\qquad - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))))))) + \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)))))))) }_{=(\mathrm{J}\odot A^4)(\mathrm{I}\odot A^2) - A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^3) - (\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)} \\
&\qquad + (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^3) - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3) + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) + A(\mathrm{I} \odot A^5) \\
&= \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))))))) + (\mathrm{J} \odot A^4)(\mathrm{I} \odot A^2) \\
&\qquad - 2A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3) - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) + (\mathrm{J} \odot A^3)(\mathrm{I} \odot A^3) \\
&\qquad + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^4) + A(\mathrm{I} \odot A^5).
\end{aligned} \tag{40}
$$

Second, we have from equality (30)

$$
\begin{aligned}
\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot ((A \odot (A\mathrm{J}))A))))) &= \mathrm{J} \odot (A((\mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^2) - A(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) \\
&\qquad - \mathrm{J} \odot A^3 + A(\mathrm{I} \odot A^2))) \\
&= \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)A^2)))}_{=\mathrm{J}\odot(A^2(\mathrm{I}\odot A^2)A^2) - A(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A^2))} - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) \\
&\qquad \underbrace{\mathrm{J} \odot (A(\mathrm{J} \odot A^3))}_{=\mathrm{J}\odot A^4 - A(\mathrm{I}\odot A^3)} + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) \\
&= \mathrm{J} \odot (A^2(\mathrm{I} \odot A^2)A^2) - A(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2)) \\
&\qquad - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2) - \mathrm{J} \odot A^4 + A(\mathrm{I} \odot A^3) \\
&\qquad + (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2).
\end{aligned} \tag{41}
$$

Third, we have from equalities (31)

$$\begin{aligned}
\mathrm{J}\odot(A(\mathrm{J}\odot(A(\mathrm{J}\odot(A(A\odot(A\mathrm{J}))))))) &= \mathrm{J}\odot(A(\mathrm{J}\odot(A^2(\mathrm{I}\odot A^2)A)-A(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A)) \\
&\qquad -\mathrm{J}\odot A^3+A(\mathrm{I}\odot A^2))) \\
&= \underbrace{\mathrm{J}\odot(A(\mathrm{J}\odot(A^2(\mathrm{I}\odot A^2)A)))}_{=\mathrm{J}\odot(A^3(\mathrm{I}\odot A^2)A)-A(\mathrm{I}(A^2(\mathrm{I}\odot A^2)A))} -(\mathrm{J}\odot A^2)(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A)) \\
&\qquad -\mathrm{J}\odot A^4+A(\mathrm{I}\odot A^3)+(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2) \\
&= \mathrm{J}\odot(A^3(\mathrm{I}\odot A^2)A)-A(\mathrm{I}(A^2(\mathrm{I}\odot A^2)A)) \qquad (42)\\
&\qquad -(\mathrm{J}\odot A^2)(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A))-\mathrm{J}\odot A^4+A(\mathrm{I}\odot A^3) \\
&\qquad +(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2).
\end{aligned}$$

Fourth, we have from equality (32)

$$\begin{aligned}
\mathrm{J}\odot(A(\mathrm{J}\odot(A(A\odot((A\odot A^2)\mathrm{J}))))) &= \mathrm{J}\odot(A(\mathrm{J}\odot(A(\mathrm{I}\odot A^3)A)-\mathrm{J}\odot(A(A\odot A^2)))) \\
&= \underbrace{\mathrm{J}\odot(A(\mathrm{J}\odot(A(\mathrm{I}\odot A^3)A)))}_{=\mathrm{J}\odot(A^2(\mathrm{I}\odot A^2)A)-A(\mathrm{I}\odot(A(\mathrm{I}\odot A^3)A))} - \underbrace{\mathrm{J}\odot(A(\mathrm{J}\odot(A(A\odot A^2))))}_{=\mathrm{J}\odot(A^2(A\odot A^2))-A(\mathrm{I}\odot(A(A\odot A^2)))} \\
&= \mathrm{J}\odot(A^2(\mathrm{I}\odot A^2)A)-A(\mathrm{I}\odot(A(\mathrm{I}\odot A^3)A)) \qquad (43)\\
&\qquad -\mathrm{J}\odot(A^2(A\odot A^2))+A(\mathrm{I}\odot(A(A\odot A^2))).
\end{aligned}$$

Fifth, we have from equality (33)

$$\begin{aligned}
\mathrm{J}\odot(A((\mathrm{J}\odot A^2)\odot((A\odot A^2)J))) &= \mathrm{J}\odot(A((\mathrm{I}\odot A^3)(\mathrm{J}\odot A^2)-A\odot A^2\odot A^2)) \\
&= \underbrace{\mathrm{J}\odot(A(\mathrm{I}\odot A^3)(\mathrm{J}\odot A^2))}_{\mathrm{J}\odot(A(\mathrm{I}\odot A^3)A^2)-A(\mathrm{I}\odot A^3)(\mathrm{I}\odot A^2)} -\mathrm{J}\odot A(A\odot A^2\odot A^2) \\
&= \mathrm{J}\odot(A(\mathrm{I}\odot A^3)A^2)-A(\mathrm{I}\odot A^3)(\mathrm{I}\odot A^2) \qquad (44)\\
&\qquad -\mathrm{J}\odot A(A\odot A^2\odot A^2).
\end{aligned}$$

Sixth, we have from equality (34)

$$\begin{aligned}
\mathrm{J}\odot(A(A\odot(C_{4f}J)) &= \mathrm{J}\odot(A((\mathrm{I}\odot(AP_3))A-C_4)) \\
&= \mathrm{J}\odot(A(\mathrm{I}\odot(A(\mathrm{J}\odot A^3-A(\mathrm{I}\odot A^2)-(\mathrm{I}\odot A^2)A+A)))A) \\
&\qquad -\mathrm{J}\odot(A(A\odot A^3-A(\mathrm{I}\odot A^2)-(\mathrm{I}\odot A^2)A+A)) \\
&= \mathrm{J}\odot(A(\mathrm{I}\odot A^4)A)-\mathrm{J}\odot(A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)A) \qquad (45)\\
&\qquad -\mathrm{J}\odot(A(\mathrm{I}\odot(A(\mathrm{I}\odot A^2)A))A)+2\mathrm{J}\odot(A(\mathrm{I}\odot A^2)A) \\
&\qquad -\mathrm{J}\odot(A(A\odot A^3))+(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2)-(\mathrm{J}\odot A^2).
\end{aligned}$$

Seventh, we have from equality (35)

$$\begin{aligned}
\mathrm{J}\odot(A(P_3^*\odot(A\mathrm{J}))) &= \mathrm{J}\odot(A((\mathrm{I}\odot A^2)P_3-C_4)) \\
&= \mathrm{J}\odot(A((\mathrm{I}\odot A^2)(\mathrm{J}\odot A^3-A(\mathrm{I}\odot A^2)-(\mathrm{I}\odot A^2)A+A))) \\
&\qquad -\mathrm{J}\odot(A(A\odot A^3-A(\mathrm{I}\odot A^2)-(\mathrm{I}\odot A^2)A+A)) \\
&= \mathrm{J}\odot(A(\mathrm{I}\odot A^2)A^3)-A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^3) \qquad (46)\\
&\qquad -\mathrm{J}\odot(A(\mathrm{I}\odot A^2)A(\mathrm{I}\odot A^2))-\mathrm{J}\odot(A(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)A) \\
&\qquad +2\mathrm{J}\odot(A(\mathrm{I}\odot A^2)A)-\mathrm{J}\odot(A(A\odot A^3))+(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2)-(\mathrm{J}\odot A^2).
\end{aligned}$$

Eighth, we have

$$\begin{aligned}
\mathrm{J}\odot(AP_3^*) &= \mathrm{J}\odot(AP_3) \\
&= \mathrm{J}\odot(A(\mathrm{J}\odot A^3-A(\mathrm{I}\odot A^2)-(\mathrm{I}\odot A^2)A+A))) \\
&= \mathrm{J}\odot A^4-A(\mathrm{I}\odot A^3)-(\mathrm{J}\odot A^2)(\mathrm{I}\odot A^2)-\mathrm{J}\odot(A(\mathrm{I}\odot A^2)A)+(\mathrm{J}\odot A^2). \qquad (47)
\end{aligned}$$

Ninth, we have

$$\begin{aligned}
\mathrm{J} \odot (AC_{4f}) &= \mathrm{J} \odot (AC_4) \\
&= \mathrm{J} \odot (A(A \odot A^3 - A(\mathrm{I} \odot A^2) - (\mathrm{I} \odot A^2)A + A))) \\
&= \mathrm{J} \odot (A(A \odot A^3)) - (\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) - \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) + (\mathrm{J} \odot A^2). \qquad (48)
\end{aligned}$$

Tenth, we have

$$\mathrm{J} \odot (A(\mathrm{J} \odot ((A \odot A^2)A))) = \mathrm{J} \odot (A(A \odot A^2)A) - A(\mathrm{I} \odot ((A \odot A^2)A)). \qquad (49)$$

Eleventh, we have

$$\mathrm{J} \odot (A(\mathrm{J} \odot (A(A \odot A^2)))) = \mathrm{J} \odot (A^2(A \odot A^2)) - A(\mathrm{I} \odot (A(A \odot A^2))). \qquad (50)$$

From equalities (40) to (50) combined with $\mathrm{J} \odot (A(A \odot A^2 \odot A^2))$ and $\mathrm{J} \odot (A(A \odot A^2))$ we obtain the equivalence between $\mathrm{J} \odot (AP_5^*)$ and all those matrices.

Twelfth, we have $A^3_{i,i} = \sum_k (A \odot A^2)_{i,k}$. Thus lemma D.1 implies

$$\begin{aligned}
P_3^* \odot ((A \odot A^2)\mathrm{J}) &= (\mathrm{I} \odot A^3)P_3 - A^2 \odot C_4 \\
&= (\mathrm{I} \odot A^3)(\mathrm{J} \odot A^3) - (\mathrm{I} \odot A^3)A(\mathrm{I} \odot A^2) - (\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A + (\mathrm{I} \odot A^3)A \\
&\quad - A^2 \odot A \odot A^3 + \underbrace{A^2 \odot (A(\mathrm{I} \odot A^2))}_{=(A \odot A^2)(\mathrm{I} \odot A^2)} + \underbrace{A^2 \odot ((\mathrm{I} \odot A^2)A)}_{=(\mathrm{I} \odot A^2)(A \odot A^2)} - A^2 \odot A \\
&= (\mathrm{I} \odot A^3)(\mathrm{J} \odot A^3) - (\mathrm{I} \odot A^3)A(\mathrm{I} \odot A^2) - (\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A \qquad (51) \\
&\quad + (\mathrm{I} \odot A^3)A - A \odot A^2 \odot A^3 + (A \odot A^2)(\mathrm{I} \odot A^2) + (\mathrm{I} \odot A^2)(A \odot A^2) \\
&\quad - A \odot A^2.
\end{aligned}$$

Thirteenth, we have $(AP_4^*)_{i,i} = \sum_k (C_{5f})_{i,k}$. Thus lemma D.1 implies

$$\begin{aligned}
A \odot (C_{5f}\mathrm{J}) &= (\mathrm{I} \odot (AP_4))A - C_5 \\
&= \underbrace{(\mathrm{I} \odot (A(\mathrm{J} \odot A^4)))A}_{=(\mathrm{I} \odot A^5)A} - \underbrace{(\mathrm{I} \odot (A(\mathrm{J} \odot (A(\mathrm{I} \odot A^2)A))))A}_{=(\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)A))A} + 2\underbrace{(\mathrm{I} \odot (A(\mathrm{J} \odot A^2)))A}_{=(\mathrm{I} \odot A^3)A} \\
&\quad - \underbrace{(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2)))A}_{=(\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A^2))A} - \underbrace{(\mathrm{I} \odot (A(\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2)))A}_{=(\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A} \\
&\quad - (\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A))A - (\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3)A + 3(\mathrm{I} \odot (A(A \odot A^2)))A - A \odot A^4 \\
&\quad + A \odot (A(\mathrm{I} \odot A^2)A) + (\mathrm{I} \odot A^2)(A \odot A^2) + (A \odot A^2)(\mathrm{I} \odot A^2) \\
&\quad + A(\mathrm{I} \odot A^3) + (\mathrm{I} \odot A^3)A - 5A \odot A^2 \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (52) \\
&\quad - 2(\mathrm{I} \odot A^3)(\mathrm{I} \odot A^2)A - (\mathrm{I} \odot (A(\mathrm{I} \odot A^3)A))A + 3(\mathrm{I} \odot (A(A \odot A^2)))A \\
&\quad + A \odot (A(\mathrm{I} \odot A^2)A) + (\mathrm{I} \odot A^2)(A \odot A^2) + (A \odot A^2)(\mathrm{I} \odot A^2) + 2(\mathrm{I} \odot A^3)A \\
&\quad + A(\mathrm{I} \odot A^3) + (\mathrm{I} \odot A^3)A - 5A \odot A^2.
\end{aligned}$$

Fourteenth, we have $(A^2)_{i,i} = \sum_k A_{i,k}$. Thus lemma D.1 implies

$$\begin{aligned}
P_4^* \odot (A\mathrm{J}) &= (\mathrm{I} \odot A^2)P_4 - C_5 \\
&= (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^4) - \mathrm{J} \odot ((\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^2)A) + 2(\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) \qquad (53) \\
&\quad - (\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2)(\mathrm{I} \odot A^2) - (\mathrm{I} \odot A^2)A(\mathrm{I} \odot A^3) \\
&\quad - (\mathrm{I} \odot A^2)(\mathrm{I} \odot A^3)A + 3(\mathrm{I} \odot A^2)(A \odot A^2) - A \odot A^4 + A \odot (A(\mathrm{I} \odot A^2)A) \\
&\quad + (\mathrm{I} \odot A^2)(A \odot A^2) + (A \odot A^2)(\mathrm{I} \odot A^2) + A(\mathrm{I} \odot A^3) + (\mathrm{I} \odot A^3)A - 5A \odot A^2.
\end{aligned}$$

Fifteenth, we have $(AP_3^*)_{i,i} = \sum_k (C_{4f})_{i,k}$. Thus lemma D.1 implies

$$\begin{aligned}
(\mathrm{J} \odot A^2) \odot (C_{4f}\mathrm{J}) &= (\mathrm{I} \odot (AP_3))(\mathrm{J} \odot A^2) - (\mathrm{J} \odot A^2) \odot C_4 \\
&= \underbrace{(\mathrm{I} \odot (A(\mathrm{J} \odot A^3)))(\mathrm{J} \odot A^2)}_{=(\mathrm{I}\odot A^4)(\mathrm{J}\odot A^2)} - (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))(\mathrm{J} \odot A^2) \\
&\quad - \underbrace{(\mathrm{I} \odot (A^2(\mathrm{I} \odot A^2)))(\mathrm{J} \odot A^2)}_{=(\mathrm{I}\odot A^2)(\mathrm{I}\odot A^2)(\mathrm{J}\odot A^2)} + (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - A^2 \odot A \odot A^3 \\
&\quad + \underbrace{(\mathrm{J} \odot A^2) \odot ((\mathrm{I} \odot A^2)A)}_{=(\mathrm{I}\odot A^2)(A\odot A^2)} + \underbrace{(\mathrm{J} \odot A^2) \odot (A(\mathrm{I} \odot A^2))}_{=(A\odot A^2)(\mathrm{I}\odot A^2)} - A^2 \odot A \\
&= (\mathrm{I} \odot A^4)(\mathrm{J} \odot A^2) - (\mathrm{I} \odot (A(\mathrm{I} \odot A^2)A))(\mathrm{J} \odot A^2) \qquad (54) \\
&\quad - (\mathrm{I} \odot A^2)(\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) + (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) - A \odot A^2 \odot A^3 \\
&\quad + (\mathrm{I} \odot A^2)(A \odot A^2) + (A \odot A^2)(\mathrm{I} \odot A^2) - A \odot A^2.
\end{aligned}$$

And eventually, from the previous equality, we have

$$A \odot A^2 \odot P_3^* = A \odot A^2 \odot A^3 - (\mathrm{I} \odot A^2)(A \odot A^2) - (A \odot A^2)(\mathrm{I} \odot A^2) + A \odot A^2, \qquad (55)$$

and

$$C_{4f}A = \mathrm{J} \odot ((A \odot A^3)A) - \mathrm{J} \odot (A(\mathrm{I} \odot A^2)A) - (\mathrm{I} \odot A^2)(\mathrm{J} \odot A^2) + \mathrm{J} \odot A^2, \qquad (56)$$

By removing the correct combination of $\mathrm{J} \odot (AP_5^*)$ and equations (51) to (56) to P_6, we obtain exactly $P_4^* + C_{5f} + 3\mathrm{J} \odot ((A \odot A^2)(\mathrm{J} \odot A^2)) + \mathrm{J} \odot A^2 \odot A^2 \odot A^2 + 3\mathrm{J} \odot ((A \odot A^2 \odot A^2)A) - 4\mathrm{J} \odot A^2 \odot A^2 - 8A \odot (A(A \odot A^2)) - 8A \odot ((A \odot A^2)A) - 4\mathrm{J} \odot ((A \odot A^2)A) - 3A \odot ((A \odot A^2)\mathrm{J}) + 17A \odot A^2 + 3\mathrm{J} \odot A^2$. It concludes the proof. □

An alternative understanding of how P_6^* computes the number of 5-paths connecting two nodes can be described as follows:

The expression AP_6^* calculates, from a given node, a non-closed 5-path followed by a 1-path. This computation inherently includes non-closed 6-paths as well as 6-cycles. The 6-cycles are subsequently removed by the Hadamard multiplication with J, which zeroes out the diagonal elements. However, this operation also allows the possibility of traversing a 5-path and then returning to an intermediate node. To account for this and eliminate respectively paths returning to the fifth, fourth, third and second nodes of the 4-paths, we subtract the other terms in P_6^*.

Thanks to formula (26), we can derive the 7-cycle formula.

Corollary D.5.1
The following formula, denoted as C_{7f} computes the number of 7-cycles linking two nodes

$$\begin{aligned}
C_{6f} &= A \odot (AP_5^*) - C_{4f} \odot ((A \odot A^2)\mathrm{J}) - A \odot (C_{5f}\mathrm{J}) - C_{5f} \odot (A\mathrm{J}) + 2C_{5f} \qquad (57) \\
&\quad - (A \odot A^2) \odot (C_{4f}\mathrm{J}) + 4A \odot A^2 \odot P_3^* + 3A \odot ((A \odot A^2)(\mathrm{J} \odot A^2) + A \odot A^2 \odot A^2 \odot A^2 \\
&\quad + 3A \odot ((A \odot A^2 \odot A^2)A) - 4A \odot A^2 \odot A^2 - 8A \odot (A(A \odot A^2)) - 12A \odot ((A \odot A^2)A) \\
&\quad - 3A \odot ((A \odot A^2)\mathrm{J}) + 20A \odot A^2.
\end{aligned}$$

In terms of time complexity, P_6^* is more efficient than P_6. The ratio of time complexity of P_6^* over P_6 is $\frac{4}{25}$. It is directly derived from the number of matrix multiplications in both formulas. Figure 7 shows the gain of complexity of P_6^* and the ratio between the two formulas.

GRL improves the computation of path and cycle at edge-level for $l = 6$ by a factor 6.25.

We evaluated the computational time of P_3^* and P_6^* and the precomputation times of GSN on the IMDB-MULTI dataset, with the results shown in Figure 14. This analysis underscores the efficiency gains provided by the formulae.

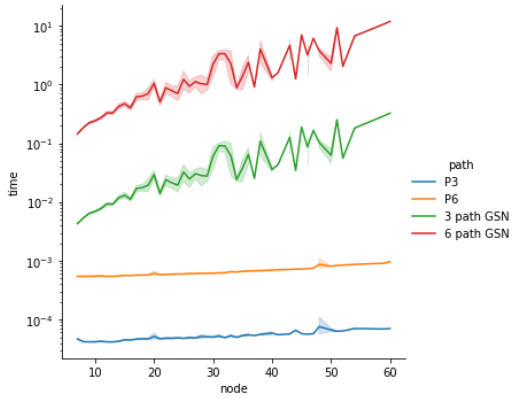


Figure 14: Time computation of GRL formulae and preconsumption of GSN (log scale) on IMDB-MULTI dataset for path of length 3 and 6.

E GRL applied on directed graphs

In this section, we extend the application of GRL to derive matrix formulae for counting paths and cycles in directed graphs.

To adapt the grammar reduction approach proposed in Piquenot et al. (2024) for directed graphs, minor modifications are necessary. Specifically, the transpose operation becomes critical due to the asymmetry of the adjacency matrix in directed graphs. Despite this adjustment, the proof used to eliminate the V_c variable remains valid. Consequently, the grammar G_d provided to GRL for this task is defined as follows.

$$\begin{aligned} E &\to (E \odot M) \mid (NE) \mid (EN) \mid E^{\mathbf{T}} \mid A \mid \mathrm{J} \\ N &\to (N \odot M) \mid (N \odot N) \mid \mathrm{I} \\ M &\to (MM) \mid (EE) \mid M^{\mathbf{T}} \end{aligned} \tag{58}$$

In addition to GRL, we explored search within the CFG using two alternative methods: MCTS without GramFormer, referred to as MC, and a completely random rule selection process, referred to as Rand. For both MC and Rand, we maintained the same rollout budget and maximum sentence length as those used for GRL. In the following, we denote the path matrix for directed graphs as P_l^d.

For $l = 2$, since the task can be resolved by a single short formula, GRL, MC, and Rand all successfully identified P_2^d.

$$P_2^d = \mathrm{J} \odot A^2.$$

For $l = 3$, when GRL was initially applied to directed graphs, we aimed to identify a combination of four sentences to construct the formula. However, GRL determined that, similar to the case of undirected graphs, only two sentences were required. This resulted in the following simplified formula.

$$P_3^d = \mathrm{J} \odot (A(\mathrm{J} \odot A^2)) - A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}).$$

Both MC and Rand failed to converge when tasked with finding a combination of four sentences. However, after GRL revealed that only two sentences were necessary, we re-evaluated MC and Rand under this condition. In this case, both methods successfully converged and identified P_3^d.

For $l = 4$, only GRL successfully discovered a solution.

$$
\begin{aligned}
P_4^d = {} & \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))) - \mathrm{J} \odot (A(A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}))) \\
& - \mathrm{J} \odot ((A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}))A) - A \odot ((A \odot (A^2)^{\mathbf{T}})\mathrm{J}) + 2 * A \odot A^{\mathbf{T}} \odot A^2.
\end{aligned}
$$

For $l = 5$, only GRL successfully discovered a solution.

$$
\begin{aligned}
P_5^d = {} & \mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot (A(\mathrm{J} \odot A^2)))))) - \mathrm{J} \odot (A(\mathrm{J} \odot (A(A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}))))) \\
& - \mathrm{J} \odot (A(\mathrm{J} \odot ((A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}))A))) - \mathrm{J} \odot (A(A \odot ((A \odot (A^2)^{\mathbf{T}})\mathrm{J}))) \\
& - (\mathrm{J} \odot A^2) \odot ((A^{\mathbf{T}} \odot A^2)\mathrm{J}) - A \odot ((A \odot (A(\mathrm{J} \odot A^2))^{\mathbf{T}})\mathrm{J}) \\
& - ((A \odot A^{\mathbf{T}})\mathrm{J}) \odot (\mathrm{J} \odot (A(\mathrm{J} \odot A^2))) - A \odot ((A \odot A^{\mathbf{T}})\mathrm{J}) - A \odot A^{\mathbf{T}} \odot ((A \odot A^{\mathbf{T}})\mathrm{J}) \\
& - A^{\mathbf{T}} \odot A^2 - 3A \odot (A \odot A^{\mathbf{T}})^2 + 2A \odot A^2 \odot +^{\mathbf{T}} A \odot A^{\mathbf{T}} \odot (A(\mathrm{J} \odot A^2))(A^2) \\
& + \mathrm{J} \odot ((A \odot (A^2)^{\mathbf{T}})A) + 2\mathrm{J} \odot ((A \odot A^{\mathbf{T}} \odot (A^2))A) \\
& + \mathrm{J} \odot ((A \odot A^{\mathbf{T}})(\mathrm{J} \odot A^2)) + ((A \odot A^{\mathbf{T}})\mathrm{J}) \odot (A \odot ((A \odot A^{\mathbf{T}})\mathrm{J})) \\
& + A \odot (((A \odot A^{\mathbf{T}}) \odot ((A \odot A^{\mathbf{T}})\mathrm{J}))\mathrm{J}) + 2 * \mathrm{J} \odot (A(A \odot A^{\mathbf{T}} \odot A^2)).
\end{aligned}
$$

To the best of our knowledge, the matrix formulae derived for counting paths of lengths 2 to 5 are novel. This highlights the capability of GRL to generate new and meaningful formulae. Furthermore, when assuming that the adjacency matrix A is symmetric, the formulae discovered by GRL for directed graphs align perfectly with those identified for undirected graphs. This alignment leads us to conjecture that GRL has identified optimal formulae, at least in the undirected case.

F Algorithms

This section provides the pseudo code of algorithm of section 2 through 4.

Algorithm 1: PDA sentence generation for a given grammar G.

```
Input:
  The PDA (Q, Σ, Γ, δ, q_0, Z, F) derived from a given CFG G.
Output:
  A sentence w ∈ L(G) where each element of w is in Σ.
Initialisation:
  S ← [Z] # Initialisation of the stack
  w ← [ ] # Initialisation of the written sentence
while S ≠ [ ] do
  c ← pop(S)
  if c ∈ Σ then
    Append c to w # Write the terminal symbol c
  else
    Choose t ∈ δ(q_0, ε, c) # Choose a transposition for the variable c
    push(S, t) # Concatenate the rule t to the stack
Return: w
```

Algorithm 2: Definition of the algorithm *read*, that return the first variable token in input I and its position if I contains variable token

Input:
- The set of token $T := \{T_v, T_r, T_t\}$ derived from a given CFG G
- The Input I, concatenation of $w \in \Sigma^*$ the written terminal symbols with the stack $S \in \Gamma^*$

Output:
- b a boolean that indicate whether I contains elements of the variables token set T_v
- $v \in T_v$ a variable token, None if b is False
- pos the position of v in I, None if b is False

Initialisation:
- $b \leftarrow False$ $v \leftarrow None$ $pos \leftarrow None$

for $c, i \in enumerate(I)$ **do**
- **if** $c \in T_v$ **then**
  - $b \leftarrow True$
  - $v \leftarrow c$
  - $pos \leftarrow i$
  - Break

Return : b, v, pos

Algorithm 3: Prediction algorithm of the gramformer model $M = (encoder, decoder)$.

Input:
- A variable token $v \in T_v$ of the set of token $T := \{T_v, T_r, T_t\}$ derived from a given CFG G
- A variable mask M_v corresponding to the variable token v
- The Input I, concatenation of $w \in \Sigma^*$ the written terminal symbols with the stack $S \in \Gamma^*$

Output:
- *policy* the learned distribution of possible rules selection form the variable corresponding to v
- optional:*value* the learned empirical value

$memory \leftarrow encoder(v)$
$latent \leftarrow decoder(memory, I)$
$value \leftarrow MLP(latent, 1)$ # Optional
$pol \leftarrow MLP(latent, nbtoken)$
$policy \leftarrow softmax(pol + M_v)$ # probability distribution of the possible transposition of token variable v
Return : *policy*,(*value* # Optional)

Algorithm 4: *Replace* the variable of I at position *pos* by the list of variable and/or terminal tokens corresponding to the rule token at indices *decision*

Input:
- The Input I, concatenation of $w \in \Sigma^*$ the written terminal symbols with the stack $S \in \Gamma^*$
- The position of the variable token to replace *pos*
- The indice *decision* of the selected rule token

Output:
- A new I where, the variable at position I as been replaced by the list of variable and/or terminal tokens corresponding to the rule token at indices *decision*

$sb \leftarrow I[: pos]$
$sf \leftarrow I[pos + 1 :]$
$si \leftarrow tokens(decision)$
Return : $concatenate(sb, si, sf)$

Algorithm 5: Gramformer sentence generation for a given grammar G.

Input:
The transformer model M, the set of token $T := \{T_v, T_r, T_t\}$ and the dictionary of variable mask M_v derived from a given CFG G.

Output:
A sentence $w \in L(G)$ where each element of w is in Σ.

Initialisation:
$I \leftarrow [Z]$ # Initialisation of the input
$b, v, pos \leftarrow read(I)$ # read the input

while b **do**
$policy \leftarrow M(v, M_v[v], I)$ # Distribution proposed by the transformer model
$decision \leftarrow argmax(policy)$
$I \leftarrow replace(I, pos, decision)$
$b, v, pos \leftarrow read(I)$

Return : I

Algorithm 6: GRL algorithm one agent acting phase

Input:
A $MCTS$ defined to search within a CFG G
$nbwords$, the number of sentences to generate
A fixed Gramformer M
A $buffer$

Output:
A $buffer$ that contains empirical policy and value of the tree explored during MCTS for the selected nodes of this MCTS.

Initialisation:
$I \leftarrow [Z] * nbwords$ # Initialisation of the input
$b, v, pos \leftarrow read(I)$ # read the input
$tree \leftarrow initMCTS(nbwords)$
$buffer \leftarrow [I]$

while b **do**
$root \leftarrow tree(I)$
$decision, tree \leftarrow MCTS(root, M)$
$I \leftarrow replace(I, pos, decision)$
$b, v, pos \leftarrow read(I)$
Append I to $buffer$

Return : fill$(buffer, tree)$

Algorithm 7: MCTS algorithm

Input:
The gramformer model M, and $root$, a node of the tree.

Output:
A $child$ of the root node guided by the MCTS heuristic.

for *i=1 to N (Number of simulations)* **do**
$leaf \leftarrow selection(root, M)$
$child \leftarrow Expansion(leaf)$
$reward \leftarrow simulation(child)$
$Backpropagation(child, reward)$

Return : $Bestchild(root, M)$

Algorithm 8: MCTS selection step

Input:
The gramformer model M and a *node* of the tree
Output:
A descendant node of the input *node* guided by the MCTS heuristic.
while *node is fully expanded and not leaf* **do**
$node \leftarrow Bestchild(node, M)$
Return : *node*

Algorithm 9: MCTS expansion step

Input:
a *node* of the tree
Output:
A descendant node of the input *node* or the input *node*.
if *node is not leaf and not fully expanded* **then**
$node \leftarrow RandomUnvisitedChild(node)$
Return : *node*

Algorithm 10: MCTS simulation step

Input:
a *node* of the tree
Output:
A reward.
while *node is not leaf* **do**
$node \leftarrow RandomAction(node)$
Return : $Evaluate(node)$

Algorithm 11: MCTS backpropagation step

Input:
a *node* of the tree, a *reward*.
while *node is not root* **do**
Add 1 to the visit count of *node*
Add *reward* to the reward count of the *node*
$node \leftarrow$ parent of *node*

Algorithm 12: MCTS bestchild algorithm

Input:
The gramformer model M and a *node* of the tree
Output:
The best child of *node*.
$policy, - \leftarrow M(node)$
$N \leftarrow$ visits count of *node*
$res \leftarrow \{\ \}$
for *child of node* **do**
$-, reward \leftarrow M(child)$
$N_c \leftarrow$ visits count of *child*
$v \leftarrow M(child)$
$Q \leftarrow$ value of *child* / visits count of *child*
$res[child] \leftarrow \alpha Q + (1-\alpha)v + c \times policy(child) \times \frac{\sqrt{\sum_c N_c}}{1+N}$
Return : $argmax(res)$

Algorithm 13: GRL learning phase algorithm

```
Input:
    The gramformer model M and a buffer containing policy and value for given
      nodes of former trees.
Output:
    The updated gramformer M
optimiser ← ADAM(M, lr)
for i=1 to N (number of epoch) do
    for node in buffer do
        policy, reward ← M(node)
        policyLoss ← KLLoss(policy,policy of node)
        valueLoss ← HubertLoss(reward,value of node)
        Loss ← policyLoss + valueLoss
        backward(Loss)
        step of optimser
Return: M
```