Abstract

Background: Network motif algorithms have been a topic of research mainly after the 2002-seminal paper from Milo et al, that provided motifs as a way to uncover the basic building blocks of most networks. In Bioinformatics, motifs have been mainly applied in the field of gene regulation networks field.

Results: This paper proposes new algorithms to exactly count isomorphic pattern motifs of sizes 3, 4 and 5 in directed graphs.

Let $G(V, E)$ be a directed graph with $m = |E|$. We describe an $O(m \sqrt{m})$ time complexity algorithm to count isomorphic patterns of size 3. In order to count isomorphic patterns of size 4, we propose an $O(m^2)$ algorithm. To count patterns with 5 vertices, the algorithm is $O(m^2 n)$.

Conclusion: The new algorithms were implemented and compared with FANMOD and Kavosh motif detection tools. The experiments show that our algorithms are expressively faster than FANMOD and Kavosh's. We also let our motif-detecting tool available in the Internet.

keywords: network motifs, complex networks, algorithm design and analysis, counting motifs, detecting motifs, motifs, discovery, motif isomorphism.

1 Background

Network Motifs, or simply motifs, correspond to small patterns that recurrently appear in a complex network [2]. They can be considered as the basic building blocks of complex networks and their understanding may be of interest in sev-
eral areas, such as Bioinformatics [10,12], Communication [25], and Software Engineering [11].

Finding network motifs has been a matter of attention mainly after the 2002-seminal paper from Milo et al. [16], that proposed motifs as a way to uncover the structural design of complex networks. Nowadays, the design of efficient algorithms for network motif discovery is an up-to-date research area. Several surveys about motif detection algorithms were published in recent years [6,21,24].

1.1 Problem statement

This paper formally addresses the following three problems:

**Problem 1.1 (Motifs-3)** Given a directed graph \( G(V, E) \), the problem Motifs-3 consists in counting the number of connected induced subgraphs of \( G \) of size 3 grouped by the 13 isomorphic distinct graphs of size 3.

**Problem 1.2 (Motifs-4)** Given a directed graph \( G(V, E) \), the problem Motifs-4 consists in counting the number of connected induced subgraphs of \( G \) of size 4 grouped by the 199 isomorphic distinct graphs of size 4.

**Problem 1.3 (Motifs-5)** Given a directed graph \( G(V, E) \), the problem Motifs-5 consists in counting the number of connected induced subgraphs of \( G \) of size 5 grouped by the 9364 isomorphic distinct graphs of size 5.

1.2 Related work and tools

The algorithms for motif detection can be based on two main approaches: exact counting or heuristic sampling. As these names might suggest, the former approach performs a precise count of the isomorphic pattern frequency. The latter uses statistics to estimate frequency value. Several exact search-based algorithms and tools can be found in the literature, such as MAVisto [22], NeMoFinder [4], Kavosh [8] and Grochow and Kellis [7]. Examples of sampling-based algorithms are MFinder [9,17], FANMOD [23] and MODA [19].

In 2010, Marcus and Shavitt [13,14] provided an exactly algorithm \( O(m^2) \) to count network motifs of size 4 in undirected graphs. In Section 2.4 Figure 3 shows the only six connected isomorphic patterns with 4 vertices, that can be labeled as: tailed triangle, 4-cycle, 4-cycle with chord, 4-clique, 4-path and Claw. In fact, the paper provided six independent algorithms; each one devoted to count an undirected isomorphic pattern. Some ideas of Marcus and Shavitt are present in our approach. However, this paper provides a solution to directed graph cases. Furthermore, this work also solves 5-sized motifs. A short version of this paper of this work appears in [15].

1.3 Our approach: combinatorial acceleration

This paper presents faster exact algorithms to Motif-3, Motif-4 and Motif-5 problems. Basically, two main techniques are applied to improve computational
complexity: first, our algorithm compute the number of isomorphic patterns instead of listing induced subgraphs; second, our method does not actually check isomorphism. The algorithms associate an integer variable with each isomorphic pattern and increment it directly.

Our algorithm was evaluated on transcription of biological networks (bacteria E. coli and the yeast S. cerevisiae) and public dataset networks with up to 13,000 vertices and 100,000 edges. The results are summarized on Tables 8, 9 and 10. Such tables show a significant improvement in performance for Motif-3, Motif-4 and Motif-5. The acc-Motif was able to solve instances considered unfeasible in the current programs, which takes several days to be solved even in probabilistic models.

We believe that the technique can be extended for detecting motifs of higher sizes.

The program was implemented in Java and it is made available as freeware in http://www.ft.unicamp.br/~meira/accmotifs.

1.4 Paper organization

The remaining of this paper is organized as follows: Section 2 describes the implemented algorithms; Section 2.1 depicts the notation used, Section 2.2 introduces the new approach starting by the simple case of counting isomorphic patterns of size 3, and Sections 2.4 and 2.5 show the method applied to counting isomorphic patterns of size 4 in undirected and directed graphs, respectively. Subsections 2.6 and 2.7 are dedicated to count isomorphic patterns of size 5. Section 3 presents the computational results, in comparison to other well-known tools available. Finally, Section 4 presents the conclusion and our view of future work.

2 Implementation

The existing exact algorithms to find network motifs are generally extremely costly in terms of CPU time and memory consumption, and present restrictions on the size of motifs [8]. According to Cirielo and Guerra [6], motif algorithms typically consist of three steps: (i) listing connected subgraphs of $k$ vertices in the original graph and in a set of randomized graphs; (ii) grouping them into isomorphic classes; and (iii) determining the statistical significance of isomorphic subgraph classes by comparing their frequencies to those of an ensemble of random graphs. The core of this paper focuses on items (i) and (ii).

Section 2.1 presents the notation in use. Section 2.2 describes the algorithm to Motif-3 problem. Sections 2.4 and 2.5 describe the algorithm to Motif-4 problem. Sections 2.6 and 2.7 describe the algorithm to Motif-5 problem.
2.1 Notation and definitions

Let $G(V, E)$ be a directed graph with $n = |V|$ vertices and $m = |E|$ edges. Assuming that $m \geq n - 1$. If $(u, v) \in E$ and $(v, u) \in E$, we say it is a bidirected edge. Alternatively, if only $(u, v) \in E$, we say it is a directed edge.

Given a vertex $v \in V$, we partitioned the neighbors of $v$ in three disjoint sets: $\delta^+(v)$, $\delta^+(v)$ and $\delta^-(v)$, as follows:

$$u \in \begin{cases} 
\delta^+(v), & \text{if } (u, v) \in E \text{ and } (v, u) \in E \\
\delta^{-}(v), & \text{if } (u, v) \in E \text{ and } (v, u) \not\in E \\
\delta^{-}(v), & \text{if } (u, v) \in E \text{ and } (v, u) \not\in E
\end{cases}$$

It means that $\delta^+(v)$ are the vertices with a bidirected edge to $v$. The vertices with edges directed from $v$ are in $\delta^+(v)$ and the vertices with edges directed to $v$ are in $\delta^-(v)$.

Sometimes, for convenience, we consider an undirected version of $G(V, E)$ called $G^+(V, E^+)$ where $(u, v) \in E^+$ if and only if $(u, v) \in E$ or $(v, u) \in E$, or both. Therefore, we replace directed or bidirected edges of $G$ by a single undirected edge in $G^+$. Let us define $\delta(v)$ as the neighbors of $v$, thus $u \in \delta(v)$ if and only if $(u, v) \in E^+$. Note that $\delta(v) = \delta^+(v) \cup \delta^-(v)$.

Given two disjoint sets $A \subseteq V$ and $B \subseteq V$, we define $\delta^+(A, B)$ as the set of bidirected edges between the sets $A$ and $B$ and $\delta^+(A, B)$ as the directed edges from $A$ to $B$. We also define $\delta^+(A, A)$ for a single set $A$ as the bidirected edges $(u, v)$ with $u \in A$ and $v \in A$ and $\delta^+(A, A)$ as directed edges with $u \in A$ and $v \in A$.

We define the adjacency of a set of vertices $V' \subseteq V$ as $\text{adj}(V') = \{ \cup_{v \in V'} \delta(v) \} \setminus V'$.

2.2 Counting isomorphic patterns of size 3

To simplify notation usage, Table 2 defines a set of auxiliary variables related to a vertex $v$.

The symbol $A^v = \delta^+(v)$ represents the set of bidirected neighbors of $v$, $B^v = \delta^+(v)$ is the set of directed neighbors from $v$, and $C^v = \delta^-(v)$ is the set of directed neighbors to $v$. The sets $A^v$, $B^v$ and $C^v$ define a partition of vertices in $v$ adjacency. For simplicity of notation, if the vertex $v$ is clear the superscript of $v$ can be removed.

The number of bidirected neighbors of $v$ is given by $n^v$. The number of directed edges from $A^v$ to $B^v$ is $m_{ab}^v$. The notation $m^l$ is used to represent the number of bidirected edges, for example, $m_{ab}^l$ is the number of bidirected edges between $A$ and $B$ and $m_{aa}^l$ is the number of bidirected edges inside $A^v$.

The algorithm to count 3-sized motifs is derived from Theorem 2.2. However, in order to provide it with a better understanding, the following definition is needed:

**Definition 2.1 (v-Patterns)** Given a directed graph $G(V, E)$, we define $v$-Patterns, for any $v \in V$, as a set of induced subgraphs with three vertices,
\{v, x, y\}, where \(x\) and \(y\) are in \(\delta(v)\), which means all induced subgraphs with the vertex \(v\) and more two vertices in its adjacency. The same definition is valid for the case of undirected graph.

To illustrate the combinatorial optimization technique used in this paper, let us start by analyzing a simple case. Consider a star graph \(G^S(V^S, E^S)\) with center \(v_c\) and neighbors \(A^{v_c}, B^{v_c}\) and \(C^{v_c}\) as described in Figure 1.

| Pattern          | Frequency       |
|------------------|-----------------|
| \(o \leftrightarrow o \rightarrow o\) | \(n_a^{v_c} n_b^{v_c}\) |
| \(o \leftrightarrow o \leftarrow o\)   | \(n_a^{v_c} n_c^{v_c}\) |
| \(o \rightarrow o \rightarrow o\)     | \(n_b^{v_c} n_c^{v_c}\) |
| \(o \leftrightarrow o \leftrightarrow o\) | \(2 n_a^{v_c}\) |
| \(o \leftarrow o \rightarrow o\)     | \(2 n_b^{v_c}\) |
| \(o \rightarrow o \leftarrow o\)     | \(2 n_c^{v_c}\) |

Figure 1: Star graph and its sets. Isomorphic pattern frequencies on the right.

A naive algorithm to motif counting will compute all vertices in \(\delta(v_c)\) combined two by two. We argue that it is possible to compute the isomorphic patterns in \(G^S\) in constant time \(O(1)\), since we have precomputed the auxiliary variables of Table 1.

Figure 1 brings an insight about how our algorithm works. It shows, in a simple example, that it is possible to count isomorphic patterns without explicit listing all of them. The right side of the figure depicts all possible patterns and occurrence frequencies in the star graph \(G^S\). It is possible to achieve, for instance, a number of exactly \(n_a^{v_c} n_b^{v_c}\) occurrences of pattern “\(o \leftrightarrow o \rightarrow o\)”, which means a pattern with a center vertex linked to the left neighbor vertex by a bidirected edge and linked to the right neighbor by an edge directed to it.

The algorithm to count isomorphic patterns in a general graph derives from the following theorem.

**Theorem 2.2** Let \(G(V, E)\) be a general graph and \(v\) any vertex in \(V\). The patterns occurrences in set \(v\)-Patterns are given by Table 2.

**Proof.**

This theorem is proved by induction. Observe that the \(v\)-Patterns set considers the patterns containing \(v\) and two vertices in \(\delta(v)\). Let \(G'(E', V')\) be the graph \(G\) induced by \(v \cup \delta(v)\). The basic case is if the \(G'\) is a star graph. In this case, the \(v\)-Patterns frequencies are equal to Figure 1 on the right. Table 2 corresponds to it if all \(m^v\) variables are zero, which is the case in \(G'\).
Suppose that a new \((x, y)\) directed edge is added to \(G'\) where \(x\) and \(y\) are in \(\delta(v)\). The new graph has edges \(E' \cup \{u, v\}\). At this moment, our sole interest is devoted to subgraph patterns that contain the vertex \(v\).

The number of pattern \(\rightarrow \leftrightarrow \rightarrow\) in the original \(G'\) is \(n^v_b n^v_c\). If the new directed edge \((x, y)\) has \(x \in C^v\) and \(y \in B^v\), one pattern \(\rightarrow \leftrightarrow \rightarrow\) is removed and a cyclic pattern is added. The added pattern is shown in Table 2, Line 13.

If \(u \in A\) and \(v \in A\) one pattern \(\leftrightarrow \leftrightarrow \rightarrow\) is removed and another is added. The added pattern is shown in Table 2, Line 11. For each edge added in \(\delta(v)\), one pattern containing \(v\) is removed and another pattern containing \(v\) is added.

A straightforward generalization is observed for an arbitrary number of added edges. Suppose \(m^v_{c,b}\) directed edges are added from \(C^v\) to \(B^v\). The number of \(\rightarrow \leftrightarrow \rightarrow\) decreases \(m^v_{c,b}\) units and exactly \(m^v_{c,b}\) occurrences arise from a new one, which can be seen in Table 2, Line 13.

Thus, given a graph \(G(V, E)\), for each vertex \(v \in V\), it is possible to obtain the \(v\)-Patterns frequencies using Theorem 2.2. Table 2 shows this pattern frequency (see variable definition in Table 1).

If the variables of Table 1 were preprocessed, it is possible to calculate all isomorphic patterns of size 3 containing a vertex \(v \in V\) and two other neighbors of \(v\) in \(O(1)\).

The pattern containing \(v\), a neighbor of \(v\), and a non-neighbor of \(v\) will be ignored by the \(v\)-Patterns set. Fortunately, valid patterns involving these vertices could be computed by their center vertex at another moment. Patterns related to \(C_3\) will be considered three times each. The pattern \(C_3\) is in the \(v\)-Patterns set of vertices \(v_1, v_2\) and \(v_3\) in \(C_3\). Therefore, a simple correction must be applied. The final counter of \(C_3\) related isomorphic patterns must be divided by three to provide the correct value.

The Algorithm 1 counts motifs patterns of size 3. In fact, the algorithm does not perform any isomorphic matching. The algorithm creates a vector \(h\) with thirteen integers and initializes them with zero. In this vector, the pattern \(\leftrightarrow \leftrightarrow \rightarrow\) is arbitrarily associated with \(h[0]\), the pattern \(\leftrightarrow \rightarrow \rightarrow\) is arbitrarily associated with \(h[1]\), \(\rightarrow \leftrightarrow \rightarrow\) with \(h[2]\), and so on. The algorithm computes Table 2 frequencies for each \(v \in V\). The frequencies of Table 2 are incremented in vector \(h\) directly. The algorithm output is vector \(h\), containing thirteen isomorphic pattern frequencies.

The complexity of the algorithm is dominated by Line 2, which computes variables in Table 1. All operations in Algorithm 1 except Line 2, are \(O(n)\). The next section shows how to compute Line 2 in \(O(m\sqrt{m})\).

### 2.3 Preprocessing Table 1

This section argues that, given a directed graph \(G(V, E)\), it is possible to compute Table 1 sets and variables in \(O(a(G)m)\), where \(a(G)\) is the arboricity of the undirected version of \(G\). Arboricity was introduced by Nash-Williams [18].
Input: Directed graph $G(V, E)$

Output: Histogram to 13 isomorphic patterns to motifs of size 3

1. Create a histogram data structure to count isomorphic patterns
2. Calculate the variables of Table 1 to all vertices.
3. foreach $v \in V$ do
   4. Calculate the number of patterns involving vertex $v$ using frequencies of Table 2
   5. For each pattern, add this frequency counter to histogram.
4. end
5. if The undirected version of the pattern is the cycle graph $C_3$ then
   6. Divide the frequency counter by 3
7. end
8. return The histogram.

Algorithm 1: Count 3 Sized Patterns Algorithm.

the arboricity $a(G)$ of a graph $G$ is the minimum number of forests into which its edges can be partitioned. It is known [5] that $a(G) = O(\sqrt{E})$ to any graph, so the execution complexity is also $O(m\sqrt{m})$.

First, for each vertex $v \in V$, create three sets $A^v, B^v$, and $C^v$. Algorithm 2 describes how to compute such variables in $O(m)$.

Input: Directed graph $G(V, E)$

Output: Variables $A^v, B^v$, and $C^v$ and $n^v_a, n^v_b, n^v_c$ for all $v \in V$

1. foreach $v \in V$ do
   2. $(A^v, B^v, C^v) \leftarrow (\emptyset, \emptyset, \emptyset)$
3. end
4. foreach bidirected $(u, v) \in E$ do
   5. $A^u \leftarrow A^u \cup \{v\}$
   6. $A^v \leftarrow A^v \cup \{u\}$
7. end
8. foreach directed $(u, v) \in E$ do
   9. $B^u \leftarrow B^u \cup \{v\}$
   10. $C^v \leftarrow C^v \cup \{u\}$
11. end
12. foreach $v \in V$ do
13. $(n^v_a, n^v_b, n^v_c) \leftarrow (|A^v|, |B^v|, |C^v|)$
14. end

Algorithm 2: Create $\{A^v, B^v, C^v\}$ variables.

Algorithm computes variables $\{m^v_{a, a}, \ldots, m^v_{c, c}\}$. The complexity is dominated by Line 5, the algorithm that lists all triangles in an undirected graph. If Chiba and Nishizek algorithm [5] is used to list all triangles, an $O(a(G)m)$ algorithm is obtained, where $a(G)$ is the arboricity of $G$.

It is possible to notice that, in essence, Algorithm is processing all triangles
Input: Directed graph $G(V, E)$
Output: Variables $\{m_{a,a}^v, \ldots, m_{c,c}^v\}$.

1 Let $G^*(V, E^*)$ be the undirected version of $G(V, E)$.
2 foreach $v \in V$ do
3 All variables in $\{m_{a,a}^v, \ldots, m_{c,c}^v\}$ start with zero.
4 end
5 List all triangles of $G^*(V, E^*)$ and save in variable $T$
6 foreach triangle $(v_1, v_2, v_3) \in T$ do
7 Let $(v, x, y) \leftarrow (v_1, v_2, v_3)$
8 Do the same to $(v, x, y) \leftarrow (v_2, v_1, v_3)$ and to $(v, x, y) \leftarrow (v_3, v_1, v_2)$
9 end

Algorithm 3: Create $\{m_{a,a}^v, \ldots, m_{c,c}^v\}$ variables.

in $G(V, E)$. Each increment in $m_{a,b}^v$ is an operation in a triangle containing $v$ and two connected neighbors. We remark the existence of more straightforward implementations of Algorithm 3 but the use of Chiba and Nishizek algorithm [5] to list all triangles as a subroutine simplifies the complexity analysis.

Thus, it is possible to conclude that the Algorithm 1, which solves the Motifs-3 problem, presents an $O(a(G)m)$ time complexity. The memory used in the algorithm is linear in relation to the memory used to represent $G(V, E)$.

2.4 Counting isomorphic patterns of size 4 in undirected graphs

To show our solution of Motif-4 problem, let us start with an undirected version of the problem. The directed case involves more details and will be considered in Section 2.5.

Similarly to the previous section, the following definition needs to be known beforehand:

Definition 2.3 (e-Patterns) Given a directed graph $G(V, E)$, we define an e-Patterns, for any $e \in E$, as a set of patterns with four vertices, $\{u, v, v_1, v_2\}$,
where \((u, v) = e\) and \(v_1\) and \(v_2\) are in \(\text{adj}(\{u, v\})\). The e-Patterns set has patterns with the edge \(e\) and more two vertices in its adjacency. The same applies to the undirected graph.

The approach to count patterns with four vertices is counting e-Patterns to all \(e \in E\). Let us define \(Z^e = \delta(u) \cap \delta(v) \setminus \{u, v\}\) as the vertices adjacent to \(u\) and \(v\), \(X^e = \delta(u) \setminus (Z^e \cup \{v\})\) as the vertices only in \(u\) adjacency, and \(Y^e = \delta(v) \setminus (Z^e \cup \{u\})\) as the vertices only in \(v\) adjacency. If the edge \(e\) is clear it can be omitted from the superscript. We define \(n^e_x\), \(n^e_y\) and \(n^e_z\) as the sizes \(|X^e|\), \(|Y^e|\) and \(|Z^e|\), respectively. See Figure 2.

The \(C_k\) is the cycle graph with \(k\) vertices, the \(S_k\) is the star graph with a center and \(k\) leaves, and the \(K_k\) is the complete graph of size \(k\). The \(K_k \setminus \{e\}\) is the complete \(K_k\) graph without an arbitrary edge \(e\). The \(P_k\) is the path graph with \(k\) vertices.

![Figure 2: Sets associated with \(e = \{u, v\}\) and e-Patterns frequency of the graph on the left.](image)

| Pattern      | Frequency          |
|--------------|--------------------|
| \(P_4\)     | \(n_x n_y\)       |
| \(x \leftrightarrow C_3\) | \((n_x + n_y)n_z\) |
| \(S_3\)     | \(\binom{n_x}{2} + \binom{n_y}{2}\) |
| \(K_4 \setminus \{e\}\) | \(n_z^2\) |

**Theorem 2.4** Let \(G(V, E)\) be a general undirected graph and \(e = \{u, v\}\) any edge in \(E\). The patterns occurrences in set e-Patterns is given by Table 3.

**Proof.** This theorem is also proved by induction in the number of edges. Let \(G'\) be the graph \(G\) induced by \(\{u, v\} \cup \text{adj}(\{u, v\})\). The basic case is if \(G'\) is the graph in Figure 2. In this case, the e-Patterns frequencies are equal to Figure 2 on the right. Table 3 corresponds to it if all \(m^e\) variables are zero, which is true for the graph at issue.

If one edge \(e'\) is added into \(X^e\), one e-Patterns \(S_3\) has to be replaced by one e-Patterns \(x \leftrightarrow C_3\). The same applies to \(Y^e\). If one edge is added to \(Z^e\), one e-Patterns \(K_4 \setminus \{e\}\) has to be replaced by one e-Patterns \(K_4\). If one edge is added between \(X^e\) and \(Y^e\), one e-Patterns \(P_4\) needs to be removed and one e-Patterns \(C_4\) must be added. If one edge is added between \(X^e\) or \(Y^e\) to \(Z^e\), one e-Patterns \(x \leftrightarrow C_3\) has to be deleted and one e-Patterns \(K_4 \setminus \{e\}\) must be added. Let \(m^e_{x, y}\) be the number of edges between sets \(X^e\) and \(Y^e\). Similarly
consider variables $m^e_{x,x}$, $m^e_{x,z}$, $m^e_{y,y}$, $m^e_{y,z}$, and $m^e_{z,z}$. Thus, Table 3 presents the $e$-Patterns frequency to $e = \{u, v\}$.

The algorithm to count isomorphic patterns of size four will sum up the $e$-Patterns frequencies for all $e \in E$.

Similarly to Section 2.2, the pattern containing $\{u, v\}$, a neighbor of $u$ or $v$ and a non-neighbor of $u$ and $v$ is not considered in $e$-Patterns set. It applies to pattern $P_4$ and a non-central edge and pattern $x \leftrightarrow C_3$ and one edge in $C_3$. Fortunately, these patterns will be considered later for other edges. An induced subgraph pattern can be considered in distinct $e$-Patterns sets. So, the final histogram needs a small correction. If a pattern appears at the $e$-Patterns set for $a$ of its edges, the number of occurrences in the final histogram must be divided by $a$.

The following fact describe this situation.

**Fact 2.5** Based on Definition 2.3 and Figure 3, the $C_4$ patterns are considered by four edges. It is in $e$-Patterns for each of its four edges. The $P_4$ is in the $e$-Patterns set only for the central edge. The $S_3$ is in $e$-Patterns for each of its three edges. The tailed triangle is in $e$-Patterns in three of its four edges. The $K_4 \setminus \{e\}$ is in $e$-Patterns for each of its five edges and $K_4$ is in $e$-Patterns in each of its six edges.

The Algorithm 4 counts 4-sized subgraphs grouped by isomorphic patterns. The complexity is dominated by Line 3, the time to calculate the needed variables. All other steps are $O(m)$.

As in the previous section, there is no isomorphism detecting algorithm. The histogram is represented by a vector $h$ with 6 positions. The algorithm associates each pattern with an arbitrary *hard coded* position in the vector. For instance, patterns $(P_4, x \leftrightarrow C_3, S_3, C_4, K_4 \setminus \{e\}, K_4)$ may be related with $(h[0], h[1], h[2], h[3], h[4], h[5])$, respectively. To sum the $e$-Patterns occurrences for a specific $e \in E$ it is sufficient to update the integer variables in the vector $h$ using Table 3 rule. The algorithm output is the histogram vector containing pattern frequencies.

The Algorithm 5 computes the needed variables, according to Line 3 of Algorithm 4. The algorithm has an $O(m)$ complexity for each $e \in E$. The
\textbf{Input}: Undirected graph $G(V, E)$

\textbf{Output}: Histogram to 6 isomorphic patterns to motifs of size 4

1. Create a histogram to count isomorphic patterns

2. \textbf{foreach} $e \in E$ \textbf{do}

3. \hspace{1em} Calculate variables $n_{x}^{e}, n_{y}^{e}, n_{z}^{e}, m_{x,x}^{e}, m_{x,y}^{e}, m_{x,z}^{e}, m_{y,y}^{e}, m_{y,z}^{e}, m_{z,z}^{e}$.

4. \hspace{1em} Calculate the frequency of $e$-Patterns using Table 3.

5. \hspace{1em} For each pattern, add its frequency counter to histogram.

6. \textbf{end}

7. \textbf{if} The histogram pattern is (See Fact 2.4):

8. \hspace{1em} $x \leftrightarrow C_3$ or $S_3$: Divide the frequency counter by 3

9. \hspace{1em} $C_4$: Divide the frequency counter by 4

10. \hspace{1em} $K_4 \setminus \{e\}$: Divide the frequency counter by 5

11. \hspace{1em} $K_4$: Divide the frequency counter by 6

12. \textbf{return} The histogram.

\textbf{Algorithm 4}: Count 4 Sized Patterns Algorithm.

Variables $n_{x}^{e}, n_{y}^{e}$ and $n_{z}^{e}$ are simpler so their calculus was omitted. Note that checking whether $x \in Z^{e}$ for an arbitrary vertex $x \in V$ and edge $e = \{u, v\}$ is equivalent to checking whether $(x, u) \in E$ and $(x, v) \in E$, and can be performed in $O(1)$. Checking whether $x \in X^{e}$ and $x \in Y^{e}$ is a similar procedure.

\textbf{Input}: Undirected graph $G(V, E)$ and an edges $e \in E$

\textbf{Output}: Variables $\{m_{x,x}^{e}, \ldots, m_{z,z}^{e}\}$.

1. All variables in $\{m_{x,x}^{e}, \ldots, m_{z,z}^{e}\}$ start with zero.

2. \textbf{foreach} $(x, y) \in E$ \textbf{do}

\begin{center}
\begin{tabular}{ll}
\hline
If vertices & Var to increment \\
\hline
$x \in X^{e}$ and $y \in X^{e}$ & $m_{x,x}^{e}$ \\
$x \in X^{e}$ and $y \in Y^{e}$ & $m_{x,y}^{e}$ \\
$x \in X^{e}$ and $y \in Z^{e}$ & $m_{x,z}^{e}$ \\
$x \in Y^{e}$ and $y \in Y^{e}$ & $m_{y,y}^{e}$ \\
$x \in Y^{e}$ and $y \in Z^{e}$ & $m_{y,z}^{e}$ \\
$x \in Z^{e}$ and $y \in Z^{e}$ & $m_{z,z}^{e}$ \\
\hline
\end{tabular}
\end{center}

3. \textbf{end}

4. \textbf{return} The computed variables.

\textbf{Algorithm 5}: Create $\{m_{x,x}^{e}, \ldots, m_{z,z}^{e}\}$ variables for a given $e \in E$.

We can conclude that Algorithm 4 counts 4-sized subgraphs grouped by isomorphic patterns in $O(m^2)$ in an undirected graph $G(V, E)$. Moreover, the additional memory to store the variables is $\Theta(m)$. 

11
2.5 Counting isomorphic patterns of size 4 in directed graphs

No new concept is needed to extend the previous algorithm to the directed version. However, a large number of sets and variables have to be dealt with. Variables and sets related to an edge $e$ are presented next.

Considering an edge $e = (u, v)$, it is possible to define 15 sets associated with it.

$\mathcal{T}^e = \{A_1^e, B_1^e, C_1^e, A_2^e, B_2^e, C_2^e, AA^e, AB^e, AC^e, BA^e, BB^e, BC^e, CA^e, CB^e, CC^e\}$

defined as follows (see Figure 4): $AA^e \leftarrow A^u \cap A^v$, $AB^e \leftarrow A^u \cap B^v$, $AC^e \leftarrow A^u \cap C^v$, $BA^e \leftarrow B^u \cap A^v$, $BB^e \leftarrow B^u \cap B^v$, $BC^e \leftarrow B^u \cap C^v$, $CA^e \leftarrow C^u \cap A^v$, $CB^e \leftarrow C^u \cap B^v$, and $CC^e \leftarrow C^u \cap C^v$.

We also have sets $A_1^e \leftarrow A^u \setminus (\delta(v) \cup \{v\})$, $B_1^e \leftarrow B^u \setminus (\delta(v) \cup \{v\})$ and $C_1^e \leftarrow C^u \setminus (\delta(v) \cup \{v\})$. Finally, we have $A_2^e \leftarrow A^v \setminus \delta(u)\cup\{u\}$, $B_2^e \leftarrow B^v \setminus \delta(u)\cup\{u\}$ and $C_2^e \leftarrow C^v \setminus \delta(u)\cup\{u\}$.

The sets in $\mathcal{T}^e$ make a partition of $e$ adjacency. For instance, a vertex in $v_1 \in B_1^e$ belongs to an outside edge from $u$, a vertex $v_2 \in C_2^e$ belongs to an inside edge to $v$. A vertex in $v_3 \in AB^e$ belongs to a bidirected edge to $u$ and an outside edge from $v$.

Given a set $T \in \mathcal{T}^e$, we define $n_T^e$ as $|T|$. Given two sets $T_i, T_j \in \mathcal{T}$, we define $m_{T_i, T_j}^e$ as the number of directed edges from $T_i$ to $T_j$ and $m_{T_i, T_j}^b$ as the number of bidirected edges between $T_i$ and $T_j$. In other words, for all $T_i, T_j \in \mathcal{T}$, $m_{T_i, T_j}^e \leftarrow |\delta^+(T_i, T_j)|$ and $m_{T_i, T_j}^b \leftarrow |\delta^*(T_i, T_j)|$. Thus, if $T_i = AA^e$ and $T_j = AA^e$, then $m_{AA, AA}^e$ is the number of directed edges inside $AA^e$. If $T_i = A_1^e$ and $T_j = A_2^e$, then $m_{A_1, A_2}^e$ is the number of bidirected edges between $A_1^e$ and $B_2^e$.

Preprocessing these variables is the core technique used to accelerate our algorithm. The variables are processed only once, then they are used to infer the occurrence of motifs.
Consider an edge $e = (u, v)$ and its neighbor sets; for each $e \in E$, the algorithm will analyze and count the $e$-Patterns (see Definition 2.3). The patterns containing edge $e$ and a vertex not linked to $e$ are ignored by the $e$-Patterns set. Fortunately, all patterns are considered at least by one of its edges, as discussed in Figure 3. Patterns that are considered in more than one $e$-Patterns must to be corrected at the end of the algorithm as in the undirected case.

Consider a simple graph $G'$ as $G(V, E)$ induced in $\{u, v\} \cup \delta(u) \cup \delta(v)$. Consider no edges between $\delta(u)$ and $\delta(v)$. This graph is similar to Figure 4. Note that the set $e$-Patterns contains vertices $\{u, v\}$ plus two vertices $\{v_1, v_2\}$ in $\delta(u) \cup \delta(v)$.

Assume that $(u, v)$ is bidirected. To discover the pattern associated with $\{u, v, v_1, v_2\}$, it is sufficient to know which sets in $T^e$ are associated with $v_1$ and $v_2$. For instance, if $v_1 \in A_1$ and $v_2 \in A_3$, the associated pattern is $S_3$. If $v_1 \in AA^e$ and $v_2 \in AA^e$, the associated pattern is $K_4 \setminus \{e\}$. Let $\text{pattern}(T_i, T_j)$ for all $T_i, T_j \in T^e$ be the pattern related to $(u, v, v_1, v_2)$, where $e = (u, v)$ and $v_1 \in T_i$ and $v_2 \in T_j$. The $\text{pattern}(T_i, T_j)$ for all $T_i$ and $T_j$ is shown in Table 3.

The algorithm requires the following fact:

**Fact 2.6** Let $G'$ be any graph containing a bidirected edge $e = (u, v)$ more vertices in $(u, v)$ adjacency. Assume there are no edges in $\delta(u) \cup \delta(v)$. If it is considered a pattern $\{u, v, v_1, v_2\}$, where $v_1, v_2$ belong to the same set $T \in T^e$, there are $\binom{n_T}{2}$ occurrences of $\text{pattern}(T, T)$. If $v_1 \in T_i$ and $v_2 \in T_j$ for distinct $T_i, T_j \in T^e$, there are $n_{T_i}n_{T_j}$ occurrences of $\text{pattern}(T_i, T_j)$. More formally, the frequency of pattern $P$, $\text{freq}(P)$, containing $\{u, v\}$ in $G'$ is

$$\text{freq}(P) = \sum_{T \in T^e: \text{pattern}(T, T) = P} \binom{n_T}{2} + \sum_{T_i, T_j \in T^e: i < j, P = \text{pattern}(T_i, T_j)} n_{T_i}n_{T_j}.$$ 

It is necessary to define variations of matrix $\text{pattern}(T_i, T_j)$. If a directed edge $(v_1, v_2)$ is added in $(u, v)$ adjacency, where $v_1 \in T_i$ and $v_2 \in T_j$, one pattern is removed and one pattern is created. The removed pattern is defined as $\text{pattern}(T_i, T_j)$ and the created pattern is defined as $\text{pattern}^+(T_i, T_j)$. If edge $(v_1, v_2)$ is bidirected, the created pattern is defined as $\text{pattern}^+(T_i, T_j)$. If $v_1 \in T_j$ and $v_2 \in T_i$, the created pattern is $\text{pattern}^-(T_i, T_j)$. Figure 5 shows the patterns created when an edge is added between $T_i = A_1^e$ and $T_j = AA$. There is a straightforward generalization to other possibilities of $T_i$ and $T_j$.

The following theorem is used by the algorithm.

**Theorem 2.7** Let $G(V, E)$ be a general directed graph and $e = (u, v)$ a bidirected edge in $E$. The patterns occurrences in set $e$-Patterns is given by the following sum:

Start all frequency patterns as zero.

**foreach** $T \in T^e$ **do**

- Increase $\text{pattern}(T, T)$ occurrence by $\binom{n_T}{2} - m_{T,T} - m'_{T,T}$
- Increase $\text{pattern}^+(T, T)$ occurrence by $m'_{T,T}$
- Increase $\text{pattern}^-(T, T)$ occurrence by $m_{T,T}$

13
Table 4 \((A_1, AA^c)\) \(\text{pattern}(A_1, AA^c)\) \(\text{pattern}^\rightarrow(A_1, AA^c)\) \(\text{pattern}^\leftrightarrow(A_1, AA^c)\) \(\text{pattern}^\leftrightarrow(A_1, AA^c)\)

Figure 5: Variations of matrix \(\text{pattern}(T_i, T_j)\) for \(T_i = A_1\) and \(T_j = AA^c\).

Proof. This theorem is also proved by induction in the number of edges. Let \(G'\) be the graph \(G\) induced by \(\{u, v\} \cup \text{adj}^\prime(\{u, v\})\). Suppose that \((u, v)\) is bidirected. The basic case is if \(G'\) does not contain edge in \(\text{adj}^\prime(\{u, v\})\). In this case, the \(e\)-Patterns frequencies are given, by construction, by Fact 2.6. The proposed sum is equal to Fact 2.6 if all \(m^e\) variables are zero, which is the case for the graph at issue.

If one directed edge \((v_1, v_2)\) is added into \(T \in \mathcal{T}^e\), one occurrence of \(\text{pattern}(T, T)\) is removed and one occurrence of \(\text{pattern}^\rightarrow(T, T)\) is added. If one bidirected edge \((v_1, v_2)\) is added into \(T \in \mathcal{T}^e\), one occurrence of \(\text{pattern}(T, T)\) is removed and one occurrence of \(\text{pattern}^\leftrightarrow(T, T)\) is added.

If one directed edge \((v_1, v_2)\) is added into two distinct sets \(T_i, T_j \in \mathcal{T}^e\), one occurrence of \(\text{pattern}(T_i, T_j)\) is removed and one occurrence of \(\text{pattern}^\rightarrow(T_i, T_j)\) is added. If the added edge is \((v_2, v_1)\), the incremented pattern occurrence is \(\text{pattern}^\leftrightarrow(T_i, T_j)\). If \((v_1, v_2)\) is bidirected, the incremented occurrence is \(\text{pattern}^\leftrightarrow(T_i, T_j)\).

If the edge \(e = (u, v)\) is directed, the pattern associated with \(\{u, v, v_1, v_2\}\) must replace the bidirected edge \((u, v)\) by a directed one. In this case, the new patterns for \(v_1 \in T_i\) and \(v_2 \in T_j\) are represented by \(\text{pattern}'(T_i, T_j)\), \(\text{pattern}^\rightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\) instead of \(\text{pattern}(T_i, T_j)\), \(\text{pattern}^\rightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\). The results are the same for a directed edge \((u, v)\).

Corollary 2.8 Let \(G(V, E)\) be a general directed graph and \(e = (u, v)\) a directed edge in \(E\). The patterns occurrences in set \(e\)-Patterns can be calculated analogous to Theorem 2.7, but using \(\text{pattern}'(T_i, T_j)\), \(\text{pattern}^\rightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\), \(\text{pattern}^\leftrightarrow(T_i, T_j)\) instead
Algorithm 6 is used to count patterns of size 4 by summing the e-Patterns for all \( e \in E \) and make a correction if the same induced has been considered many times.

**Input:** Directed graph \( G(V,E) \)

**Output:** Histogram to 199 isomorphic patterns to motifs of size 4

1. Create a histogram to count isomorphic patterns
2. **foreach** \( e \in E \) **do**
3. Calculate the sets \( X^e \) for all \( X^e \in \mathcal{T}^e \).
4. Calculate the variables \( m_{x,y} \) and \( m'_{x,y} \) for all \( X^e, Y^e \in \mathcal{T}^e \).
5. Calculate the frequency involving \( e \) and two neighbors using Lemma 2.7 or Corollary 2.8.
6. For each pattern, add this frequency counter to histogram.
7. **end**
8. if the the pattern is related to:
9. \( x \leftrightarrow C_3 \) or \( S_3 \): Divide the frequency counter by 3
10. \( C_4 \): Divide the frequency counter by 4
11. \( K_4 \setminus \{e\} \): Divide the frequency counter by 5
12. \( K_4 \): Divide the frequency counter by 6
13. return The histogram.

**Algorithm 6:** Count 4 Sized Patterns Algorithm.

As in the undirected case, no isomorphism-detecting processing is used. The resultant histogram is represented by a vector of integers \( h \) with 199 position, one for each distinct isomorphic pattern of size 4. It is necessary to preprocess matrices \( \text{pattern}(,) \), \( \text{pattern}^{-}(,) \), etc., associating each pattern with an arbitrary position in \( h \). For instance, it is possible to set the \( \text{pattern}(A1, A2) \) to \( h[0] \). The \( \text{pattern}(A1, A1) \) and \( \text{pattern}(A2, A2) \) are isomorphic so they can both be associated with \( h[1] \). As a final result, each pattern in the matrices must be hard coded in association with a position in the vector \( h \) of the histogram, which will be the program output.

The complexity of the algorithm is dominated by lines 3 and 4, since all other lines are \( O(m) \). We argue that an algorithm similar to Algorithm 5 in Section 2.4 can calculate the needed variables in \( O(m^2) \). Thus, it is possible to conclude that the proposed algorithm is an \( O(m^2) \) algorithm to calculate motifs of size 4 in a directed graph.

### 2.6 Counting 5-sized patterns in undirected graphs

In this section the strategy is extended to motifs of size 5. The following definition is required:
Definition 2.9 (P₃-Patterns) Let P₃ be the path graph with three vertices p₁, p₂, p₃ ∈ V. Given an undirected graph G(V, E), we define a P₃-Patterns for any P₃ induced in G(V, E) as a set of patterns with five vertices, \{p₁, p₂, p₃, v₁, v₂\}, where v₁ and v₂ are vertices in adj(\{p₁, p₂, p₃\}). The P₃-Patterns set has patterns with an induced P₃ plus two vertices in its adjacency.

Definition 2.10 (K₃-Patterns) Let K₃ be the clique with vertices p₁, p₂, p₃ ∈ V. Given an undirected graph G(V, E), we define a K₃-Patterns for any K₃ induced in G(V, E) as a set of patterns with five vertices, \{p₁, p₂, p₃, v₁, v₂\}, where v₁ and v₂ are in adj(\{p₁, p₂, p₃\}). The K₃-Patterns set has patterns with an induced K₃ plus two vertices in its adjacency.

The approach to count patterns with five vertices is to count P₃-Patterns and K₃-Patterns patterns to all P₃ and K₃ induced in G(V, E). The time to compute the patterns frequency in P₃-Patterns and K₃-Patterns sets is O(1), considering some preprocessed variables.

The adjacency of K₃ and P₃ will be partitioned in seven groups. See Figure [7]. Let K₃ and P₃ be composed by \{(p₁, p₂, p₃)\} and assume that p₂ is the central vertex in the P₃ case.

Let us define Z = δ(p₁) ∩ δ(p₂) ∩ δ(p₃) \ \{p₁, p₂, p₃\} as the vertices adjacent to p₁, p₂ and p₃, X₁ = δ(p₁) \ \{δ(p₂) ∪ δ(p₃)\} the vertices only in p₁ adjacency, X₂ = δ(p₂) \ \{δ(p₁) ∪ δ(p₃)\} the vertices only in p₂ adjacency, and X₃ = δ(p₃) \ \{δ(p₁) ∪ δ(p₂)\} the vertices only in p₃ adjacency. Let Y₁₂ = δ(p₁) ∩ δ(p₂) \ \{Z ∪ p₃\} be the vertices only in p₁ and p₂ adjacency, Y₁₃ = δ(p₁) ∩ δ(p₃) \ \{Z ∪ p₂\} be the vertices only in p₁ and p₃ adjacency, and Y₂₃ = δ(p₂) ∩ δ(p₃) \ \{Z ∪ p₁\} be the vertices only in p₂ and p₃ adjacency. Let Q = \{X₁, X₂, X₃, Y₁₂, Y₁₃, Y₂₃, Z\}. We define nₓ₁, nₓ₂ and nₓ₃ as the sizes |X₁|, |X₂| and |X₃|, respectively, nᵧ₁₂, nᵧ₁₃ and nᵧ₂₃ as the sizes |Y₁₂|, |Y₁₃| and |Y₂₃|, respectively, and nₓ as the size of Z. Let mₓ₁,ₓ₂ be the number of edges between sets S₁ and S₂ for all S₁, S₂ ∈ Q.

Table [7] contains the K₃-Patterns frequencies for the graph in Figure [6].

The algorithm to count isomorphic patterns derives from the following theorem.

Theorem 2.11 Let G(V, E) be a general undirected graph. The pattern occurrence in set K₃-Patterns, for any induced clique (p₁, p₂, p₃), is given by Table [7]. For any induced P₃ = (p₁, p₂, p₃), the pattern occurrence in P₃-Patterns is given by Table [7].

Proof. This theorem is similar to theorems [2,2] and [2,4]. It is also proved by induction in the number of edges.

Consider the K₃-Patterns set. To the P₃-Patterns set, the proof is the same. Let G’ be the graph G induced by \{p₁, p₂, p₃\} ∪ adj(\{p₁, p₂, p₃\}). The basic case is if G’ has no edges between vertices in the adj(\{p₁, p₂, p₃\}). This graph is similar to the graph in Figure [6]. In this case, the K₃-Patterns frequency are equal to Table [7]. Table [7] corresponds to it if all m variables are zero.
Figure 6: Sets associated with \( P_3 \) or \( K_3 \). If the dashed line is considered, \( \{p_1, p_2, p_3\} \) is a \( K_3 \), otherwise, it is a \( P_3 \).

Figure 7: The pattern \( C_5 \) is in \( P_3 \)-Patterns of \( P_3 \) in bold. It is necessary to divide the final \( C_5 \) frequency by 5.

If one edge \( e' \) is added into \( X_1 \), one \( K_3 \)-Patterns pattern has to be replaced by another. The removed pattern is in Table 6, Line 1. The pattern added is in Table 6, Line 11. The same applies to other sets in \( \{X_1, X_2, X_3, Y_{12}, Y_{13}, Y_{23}, Z\} \). If one edge is added in \( Z \), one pattern (Table 6, Line 10) has to be replaced by one \( K_5 \). If one edge is added between \( X_1 \) and \( X_3 \), one pattern needs to be removed (Table 6, Line 2) and other pattern must be added (Table 6, Line 12). Thus, by a straightforward induction in edges in \( \text{adj}(\{p_1, p_2, p_3\}) \), Table 6 presents the frequency of the set \( K_3 \)-Patterns.

The algorithm to count isomorphic patterns of size five will list all \( K_3 \) and \( P_3 \) induced in \( G(V, E) \) and summing up \( K_3 \)-Patterns and \( P_3 \)-Patterns frequencies for all induced \( K_3 \) and \( P_3 \).

An induced subgraph pattern can be considered in distinct \( K_3 \)-Patterns and \( P_3 \)-Patterns sets. Thus, the final histogram needs a small correction. If a pattern appears \( a \) times as a \( K_3 \)-Patterns or a \( P_3 \)-Patterns, the final histogram result must be divided by \( a \). For instance, it is shown that \( C_5 \) is considered in 5 distinct \( P_3 \)-Patterns. See Figure 7. The correction analysis needs to be considered for all 5-sized isomorphic patterns.

The Algorithm 7 counts subgraph patterns of size 5. In lines 2 and 3, a list of all \( P_3 \) and \( K_3 \) induced in \( G(V, E) \) is computed. Algorithm 8 does this.
Input: Undirected graph $G(V, E)$

Output: Histogram to 21 isomorphic patterns to motifs of size 5

1. Create a histogram to count isomorphic patterns
2. List all induced $K_3 = (p_1, p_2, p_3)$ and save in $K$.
3. List all induced $P_3 = (p_1, p_2, p_3)$ and save in $P$.

4. foreach $t \in K \cup P$ do
   5. Calculate sets $Q = \{X_1, X_2, X_3, Y_{12}, Y_{13}, Y_{23}, Z\}$.
   6. foreach $S_1, S_2 \in Q$ do
      7. Calculate the number of edges between $S_1$ and $S_2$, $m_{S_1, S_2}$
   8. end
   9. For each pattern, add this frequency to histogram.
10. end

11. foreach pattern in the histogram do
   12. Divide the frequency by the constant $a$, correcting the repetition in several $P_3$-Patterns and $K_3$-Patterns
13. end

14. return The histogram.

Algorithm 7: Count 5 Sized Patterns Algorithm.

task in $O(\sum_{(u,v) \in E} |\delta(u)| + |\delta(v)|)$. As $|\delta(u)| + |\delta(v)| = O(n)$, the complexity of Algorithm 8 is $O(mn)$. Note that the size of $K$ and $P$ are bounded by $\Theta(nm)$.

Algorithm 7, Line 5, consists of calculating the sets $Q = \{X_1, X_2, X_3, Y_{12}, Y_{13}, Y_{23}, Z\}$ for a single $P_3$ or $K_3$. This cost is dominated by $|\delta(p_1)| + |\delta(p_2)| + |\delta(p_3)| = O(n)$. It is a simple intersection of sets procedures and can be efficiently computed using a hash.

As in the previous section, no isomorphism detecting algorithm is used. The histogram is represented by a vector $h$ with 21 positions. The algorithm associates each pattern with an arbitrary hard coded position in the vector.

Algorithm 9 computes the needed variables, according to Line 7 of Algorithm 7. The algorithm has an $O(m)$ complexity for each induced $K_3$ and $P_3$.

We can conclude that Algorithm 7 counts isomorphic pattern motifs of size 5 in $O(m^2n)$ in an undirected graph $G(V, E)$. Moreover, the additional memory to store the variables is $\Theta(mn)$.

2.7 Counting 5-sized patterns in directed graphs

Similarly to Section 2.5, no new concept is needed to extend the previous algorithm to the directed version. Both algorithms are very similar. The main difference is that the directed case requires dealing with a large number of sets. The neighborhood of $(p_1, p_2, p_3)$ is partitioned in 63 sets. It is necessary to calculate how many edges are found between each 2,016 combinations of two such sets. The histogram vector has 9,364 positions, one for each distinct isomorphic
**Input**: Undirected graph $G(V, E)$

**Output**: The set $\mathcal{P}$ of all induced $P_3$ and $\mathcal{K}$ of all induced $K_3$ in $G(V, E)$.

1. Set $\mathcal{P} \leftarrow \emptyset$, $\mathcal{K} \leftarrow \emptyset$.
2. foreach $e = \{u, v\} \in E$ do
   3. foreach $x \in \text{adj}(\{u, v\})$ do
   4. if $(x, u, v)$ is a $P_3$ and $(x, u, v)$ is not considered yet then
      5. $\mathcal{P} \leftarrow \mathcal{P} \cup \{(x, u, v)\}$
   6. end
   7. if $(x, u, v)$ is a $K_3$ and $(x, u, v)$ is not considered yet then
      8. $\mathcal{K} \leftarrow \mathcal{K} \cup \{(x, u, v)\}$
   9. end
10. end
11. end
12. return $\mathcal{K}$ and $\mathcal{P}$

Algorithm 8: List all induced $P_3$ and $K_3$.

1. pattern. Regardless of such difficulty, the algorithm deal with sets. The number of sets or set combinations in the neighborhood of $(p_1, p_2, p_3)$ is always $O(1)$.

The following definitions are required:

**Definition 2.12** Let $\mathcal{R}$ be a set of all isomorphic patterns of size 3. The set $\mathcal{R}$ contains thirteen elements:

$$\mathcal{R} = \{ \begin{array}{c} \begin{array}{c} \begin{array}{c} p_1 \rightarrow p_2, p_1 \rightarrow p_3, p_2 \rightarrow p_3 \\ p_2 \rightarrow p_1, p_1 \rightarrow p_3, p_2 \rightarrow p_3 \\ p_2 \rightarrow p_1, p_1 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_1 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \\ p_2 \rightarrow p_1, p_2 \rightarrow p_3, p_3 \rightarrow p_2 \end{array} \end{array} \end{array} \}$$

**Definition 2.13** ($\Delta$-Patterns) Let $\Delta$ be one element in $\mathcal{R}$. Given a directed graph $G(V, E)$, we define a $\Delta$-Patterns for any $(p_1, p_2, p_3)$ induced in $G(V, E)$ and isomorphic to $\Delta$, as a set of patterns with five vertices, $\{p_1, p_2, p_3, v_1, v_2\}$, where $v_1$ and $v_2$ are vertices in $\text{adj}(\{p_1, p_2, p_3\})$. A $\Delta$-Patterns is a set of patterns with an induced $\Delta$ plus two vertices in its adjacency.

Considering a pattern $\Delta \in \mathcal{R}$, it is possible to define 63 sets associated with it. Consider three variables $\alpha, \beta$ and $\gamma$ with domain $\{A, B, C, \emptyset\}$. The variables $\alpha$, $\beta$ and $\gamma$ define the neighborhood of a given vertex with respect to $p_1$, $p_2$ and $p_3$, respectively. Consider the vertices in $\text{adj}(\{p_1, p_2, p_3\})$. The Algorithm [10] partitions such vertices in 63 sets.

The role of partition is simple. If $v \in \text{set}(A, A, A)$, it is in the set with bidirected edges to $p_1$, $p_2$ and $p_3$. If $v \in \text{set}(\emptyset, \emptyset, C)$, it is not connected to $p_1$, not connected to $p_2$ and connected to $p_3$ by a directed edge to $p_3$.

Let $\mathcal{Q} = \{ \text{set}(\alpha, \beta, \gamma) \mid \forall \alpha, \beta, \gamma \in \{A, B, C, \emptyset\} \}$. Given a set $T \in \mathcal{Q}$, we define $n_T$ as $|T|$. Given two sets $T_i, T_j \in \mathcal{Q}$, we define $m_{T_i, T_j}$ as the number
Input: Undirected graph $G(V, E)$ and a connected $(p_1, p_2, p_3) \in \mathcal{K} \cup \mathcal{P}$
Output: Variables $\{m_{x_1,x_1}, m_{x_1,x_2}, \ldots, m_{z,z}\}$.

1. All variables in $\{m_{x_1,x_1}, m_{x_1,x_2}, \ldots, m_{z,z}\}$ start with zero.
2. \textbf{foreach} $(x, y) \in E$ do
   \begin{tabular}{ll}
   If vertices & Var to increment \\
   $x \in X_1$ and $y \in X_1$ & $m_{x_1,x_1}$ \\
   $x \in X_1$ and $y \in X_2$ & $m_{x_1,x_2}$ \\
   $x \in X_1$ and $y \in X_3$ & $m_{x_1,x_3}$ \\
   $x \in X_1$ and $y \in Y_{12}$ & $m_{x_1,y_{12}}$ \\
   \vdots & \vdots \\
   $x \in Z$ and $y \in Y_{23}$ & $m_{z,y_{23}}$ \\
   $x \in Z$ and $y \in Z$ & $m_{z,z}$ \\
   \end{tabular}
3. \textbf{end}
4. \textbf{return} The computed variables.

\textbf{Algorithm 9:} Create $\{m_{x_1,x_1}, m_{x_1,x_2}, \ldots, m_{z,z}\}$ variables for a given $e \in E$.

of directed edges from $T_i$ to $T_j$ and $m'_{T_i,T_j}$ as the number of bidirected edges between $T_i$ and $T_j$. In other words, for all $T_i, T_j \in \mathcal{Q}$, $m_{T_i,T_j} \leftarrow |\delta^+(T_i, T_j)|$ and $m'_{T_i,T_j} \leftarrow |\delta^*(T_i, T_j)|$. Thus, if $T_i = \text{set}(A, A, A)$ and $T_j = \text{set}(A, A, A)$ then $m_{\text{set}(A,A,A),\text{set}(A,A,A)}$ is the number of directed edges inside $\text{set}(A, A, A)$. If $T_i = \text{set}(A, A, A)$ and $T_j = \text{set}(\emptyset, \emptyset, C)$ then $m'_{\text{set}(A,A,A),\text{set}(\emptyset,\emptyset,C)}$ is the number of bidirected edges between $\text{set}(A, A, A)$ and $\text{set}(\emptyset, \emptyset, C)$.

As in Section 2.13 preprocessing these variables is the core technique used to accelerate our algorithm. The variables are processed only once. Next, they are used to calculate the occurrence of motifs.

Consider a pattern $\Delta \in \mathcal{R}$ and its neighboring sets; for each $\Delta$ induced in $G(V, E)$, the algorithm will analyze and count the $\Delta$-Patterns (see Definition 2.13). The patterns that are considered in more than one $\Delta$-Patterns must to be corrected at the end of the algorithm, as in the undirected case.

Consider a simple graph $G'$ as $G(V, E)$ induced in $\{p_1, p_2, p_3\} \cup \text{adj}([p_1, p_2, p_3])$, where $(p_1, p_2, p_3)$ is isomorphic to $\Delta$. Consider no edges in $\text{adj}([p_1, p_2, p_3])$.

To discover the pattern associated with $\{p_1, p_2, p_3, v_1, v_2\}$, it is sufficient to known $\Delta$ and which sets in $\mathcal{Q}$ are associated with $v_1$ and $v_2$.

Let $K_3$ be the complete graph of size 3, $K_5 \setminus e$ be the complete graph of size 5 with one arbitrary bidirected edge removed and $P_n$ be the path graph with $n$ vertices. All edges in $K_3$, $K_5 \setminus e$ and $P_n$ are bidirected. For instance, if $v_1 \in \text{set}(A, A, A)$ and $v_2 \in \text{set}(A, A, A)$ and $\Delta = K_3$, the associated pattern is $K_5 \setminus e$. If $v_1 \in \text{set}(A, \emptyset, \emptyset)$ and $v_2 \in \text{set}(\emptyset, \emptyset, A)$, and $\Delta = P_3$, the associated pattern is $P_5$. Let $\text{pattern}(\Delta, T_i, T_j)$ for all $\Delta \in \mathcal{R}$ and $T_i, T_j \in \mathcal{Q}$ be the pattern related to $\{p_1, p_2, p_3, v_1, v_2\}$, where $(p_1, p_2, p_3)$ is isomorphic to $\Delta$ and $v_1 \in T_i$ and $v_2 \in T_j$. The $\text{pattern}(\Delta, T_i, T_j)$ has a simple rule to be created, but
Input: Directed graph $G(V,E)$ and an induced connected subgraph $(p_1,p_2,p_3)$

Output: The vertices in $\text{adj}([p_1,p_2,p_3])$ partitioned in 63 sets.

1. $\text{foreach } \alpha \in \{A,B,C,\emptyset\}, \beta \in \{A,B,C,\emptyset\}, \gamma \in \{A,B,C,\emptyset\} \text{ do}$
   
   2. $\text{set}(\alpha, \beta, \gamma) \leftarrow \emptyset$

3. $\text{end}$

4. $\text{foreach } v \in \text{adj}([p_1,p_2,p_3]) \text{ do}$

5. 5. $\text{if } v \in \text{A}(p_1), \alpha \leftarrow A$

6. 6. $\text{if } v \in \text{B}(p_1), \alpha \leftarrow B$

7. 7. $\text{if } v \in \text{C}(p_1), \alpha \leftarrow C$

8. 8. $\text{o.c.}, \alpha \leftarrow \emptyset$

9. 9. $\text{if } v \in \text{A}(p_2), \beta \leftarrow A$

10. 10. $\text{if } v \in \text{B}(p_2), \beta \leftarrow B$

11. 11. $\text{if } v \in \text{C}(p_2), \beta \leftarrow C$

12. 12. $\text{o.c.}, \beta \leftarrow \emptyset$

13. 13. $\text{if } v \in \text{A}(p_3), \gamma \leftarrow A$

14. 14. $\text{if } v \in \text{B}(p_3), \gamma \leftarrow B$

15. 15. $\text{if } v \in \text{C}(p_3), \gamma \leftarrow C$

16. 16. $\text{o.c.}, \gamma \leftarrow \emptyset$

17. $\text{set}(\alpha, \beta, \gamma) \leftarrow \text{set}(\alpha, \beta, \gamma) \cup \{v\}$

18. $\text{end}$

19. $\text{return } \text{set}(\alpha, \beta, \gamma) \text{ for all } \alpha, \beta \text{ and } \gamma \in \{A,B,C,\emptyset\}. \text{ The set } \text{set}(\emptyset, \emptyset, \emptyset) \text{ is empty and can be ignored.}$

Algorithm 10: Algorithm to compute sets $Q$ of a given pattern $(p_1,p_2,p_3) \in R$.

it is a matrix with $13 \times 63 \times 63$ dimensions, resulting in a matrix with 51,597 precomputed patterns.

The following fact is closely related to Fact 2.6.

Fact 2.14 Consider a graph induced in $\{p_1,p_2,p_3\}$ isomorphic to $\Delta \in R$. Let $G'$ be any graph containing an induced isomorphic pattern $\Delta \in R$ plus two vertices in $\Delta$ adjacency. Assume there are no edges in $\text{adj}([p_1,p_2,p_3])$. If it is considered a pattern $\{p_1,p_2,p_3,v_1,v_2\}$, where $v_1, v_2$ belong to the same set $T \in Q$, there are $\binom{\# T}{2}$ occurrences of pattern($\Delta,T,T$). If $v_1 \in T_i$ and $v_2 \in T_j$ for distinct $T_i, T_j \in Q$, there are $n_{T_i} n_{T_j}$ occurrences of pattern($\Delta,T_i,T_j$). More formally, the frequency of pattern $P$ contained in $\Delta$-Patterns is

$$\text{freq}(P) = \sum_{T \in Q: \text{pattern}(\Delta,T,T)=P} \binom{n_{T_i}}{2} + \sum_{T_i, T_j \in Q: i < j, \text{pattern}(\Delta,T_i,T_j)} n_{T_i} n_{T_j}.$$ 

Exactly as in Section 2.5 it is necessary to define variations of pattern $\text{pattern}(\Delta,T_i,T_j)$. If a directed edge $(v_1, v_2)$ is added in $\text{adj}([p_1,p_2,p_3])$, where $v_1 \in T_i$ and $v_2 \in T_j$, one pattern($\Delta,T_i,T_j$) is removed and another pattern is created. The created pattern is defined as pattern$^{-1}(\Delta,T_i,T_j)$. If $v_1 \in T_j$ and
\(v_2 \in T_i\), the created pattern is \(\text{pattern}^{\leftarrow}(\Delta, T_i, T_j)\). If edge \((v_1, v_2)\) is bidirected, the created pattern is defined as \(\text{pattern}^{\leftrightarrow}(\Delta, T_i, T_j)\). Figure 8 shows the patterns created when \(\Delta = P_3\) and an edge is added between \(T_i = \text{set}(A, B, \emptyset)\) and \(T_j = \text{set}(\emptyset, \emptyset, C)\). There is a straightforward generalization to other possibilities of \(T_i\) and \(T_j\) in \(Q\) and \(\Delta \in \mathcal{R}\).

The following lemma is used by the algorithm.

**Lemma 2.15** Let \(G(V, E)\) be a general directed graph and \(\Delta \in \mathcal{R}\) an induced connected graph of size 3. The patterns occurrences in set \(\Delta\text{-Patterns}\) is given by the following sum:

Start all frequency patterns as zero.

\[
\text{foreach } T \in Q \text{ do}
\]

Increase \(\text{pattern}(\Delta, T, T)\) occurrence by \((n_T^2) - m_{T,T} - m_{T,T}'\)

Increase \(\text{pattern}^{\leftrightarrow}(\Delta, T, T)\) occurrence by \(m_{T,T}'\)

Increase \(\text{pattern}^{\rightarrow}(\Delta, T, T)\) occurrence by \(m_{T,T}\)

\[
\text{end}
\]

\[
\text{foreach } T_i, T_j \in Q, i < j \text{ do}
\]

Increase \(\text{pattern}(\Delta, T_i, T_j)\) occurrence by \(n_{T_i}n_{T_j} - m_{T_i,T_j} - m_{T_i,T_j}' - m_{T_j,T_i}\)

Increase \(\text{pattern}^{\leftrightarrow}(\Delta, T_i, T_j)\) occurrence by \(m_{T_i,T_j}'\)

Increase \(\text{pattern}^{\rightarrow}(\Delta, T_i, T_j)\) occurrence by \(m_{T_i,T_j}\)

Increase \(\text{pattern}^{\leftarrow}(\Delta, T_i, T_j)\) occurrence by \(m_{T_j,T_i}\)

\[
\text{end}
\]

**Proof.** Similar to Theorem 2.7.

The Algorithm 11 counts patterns of size 5 by summing the \(\Delta\text{-Patterns}\) for all \(\Delta \in \mathcal{R}\) induced in \(G(V, E)\). The algorithm applies a correction if the same induced subgraph has been considered many times. Note that the sum in Lemma 2.15 takes \(O(1)\), assuming precomputed variables.

As in the previous cases, there is no isomorphism-detecting algorithm. It is necessary to preprocess matrices \(\text{pattern}(, , )\), \(\text{pattern}^{\rightarrow}(, , )\) and \(\text{pattern}^{\leftarrow}(, , )\) associating each pattern with an arbitrary position in the histogram. Such matrices are computed once. Every execution of acc-Motif uses the same matrices.

The complexity of the algorithm is dominated by lines 6 and 8. Algorithm 10 computes the sets \(Q\) for a given \((p_1, p_3, p_3)\) in \(O(|\delta(p_1)| + |\delta(p_2)| + |\delta(p_3)|) = O(n)\). Algorithm 11 can be also adapted to compute the required variables in \(O(m)\) for a given \((p_1, p_2, p_3)\). Since all other lines are \(O(1)\) for \(\Delta\text{-Patterns}\), we conclude that the proposed algorithm is an \(O(m^2n)\) algorithm to calculate 5-sized motifs in directed graphs.

## 3 Results and Discussion

This section compares the computational results of our algorithm, that we called acc-Motif (accelerated Motif), with FANMOD [23] and Kavosh [8]. The tools
**Input:** Directed graph $G(V, E)$

**Output:** Histogram to 9364 isomorphic patterns to motifs of size 5

1. Create a histogram to count isomorphic patterns
2. Create an empty list $L_\Delta$ for all $\Delta \in \mathbb{R}$
3. List all connected $(p_1, p_2, p_3)$ induced in $G(V, E)$ and add to the correspondent $L_\Delta$
4. **foreach** $\Delta \in \mathbb{R}$ **do**
   5. **foreach** $t \in L_\Delta$ **do**
      6. Calculate sets $Q = \{set(\alpha, \beta, \gamma) \mid \forall \alpha, \beta, \gamma \in \{A, B, C, \emptyset\}\}$.
      7. **foreach** $S_1, S_2 \in Q$ **do**
         8. Calculate the number of edges between $S_1$ and $S_2$, $m_{S_1,S_2}$
      9. **end**
   10. **end**
   11. Calculate the frequency in $\Delta$-Patterns using Lemma 2.15
12. **end**
13. **foreach** pattern in the histogram **do**
   14. Divide the frequency by the constant $a$, correcting the repetition in several $\Delta$-Patterns
15. **end**
16. **return** The histogram.

**Algorithm 11:** Count 5 Sized Patterns Algorithm.

FANMOD and Kavosh were chosen because they are two of the fastest available motif finder programs [24].

The instances were arbitrarily selected from a wide range of motif applications. They are selected from open complex network databases such as Pajek and Uri Alon datasets [1, 3]. We preprocessed the instances, removing vertices with zero neighbors.

The implemented algorithms are devised to motifs of sizes 3, 4 and 5. To ensure replicability and better evaluation, we have provided the input tested graphs and the java byte-code of implemented algorithms available at [http://www.ft.unicamp.br/~meira/accmotifs](http://www.ft.unicamp.br/~meira/accmotifs).

All the tests were performed in an Intel(R) Core(TM)2 Quad CPU Q8200, 2.33 GHz, 2 GB RAM, using an algorithm implemented in Java language. We set FANMOD and Kavosh with the full enumeration parameter. Thus, FANMOD, Kavosh and acc-Motif solve the same problem, which consists in counting all subgraph of the selected size. The final histogram is exactly the same for a given graph, ensuring the correctness of acc-Motif.

Tables 8, 9 and 10 show the execution time of FANMOD, Kavosh and acc-Motif for $k$ equal to 3, 4 and 5, respectively. The algorithm is executed in the original graph and in a set of random graphs. The number of random graphs is 100, 10 and 5 for $k$ equal to 3, 4 and 5, respectively. The time reported is the average considering the original and the random graphs. In this experiment, only the execution time is considered to enumerate all subgraphs. The time to generate the random graphs is not considered.
Each round consists in the subgraph enumeration in the original and in the random graphs. We repeated the execution by five rounds per instance. Tables 8, 9, and 10 contain the average and the deviation factor of these five measurements.

We limited the CPU time to 5 hours per graph for the sake of convenience. In tables 8, 9, and 10, it is possible to observe that the proposed algorithms were expressively faster than FANMOD and Kavosh in almost all tested instances. For \( k = 3 \) and instance Airport \[20\], acc-Motif spent 35 \( \pm \) 0.2 ms/graph, Kavosh spent 1,250 \( \pm \) 6 ms/graph and FANMOD spent 5,772 \( \pm \) 2 ms/graph. For \( k = 4 \) and instance ODLIS \[3\], acc-Motif spent 2,605 \( \pm \) 115 ms/graph, Kavosh spent 210,015 \( \pm \) 837 ms/graph and FANMOD spent 630,936 \( \pm \) 2,914 ms/graph. For \( k = 5 \) and instance California \[3\], acc-Motif spent 76 \( \pm \) 0.4 s/graph, Kavosh spent 1,532 \( \pm \) 12 s/graph and FANMOD spent 2,376 \( \pm \) 12 s/graph. The performance gain of acc-Motif was consistently observed in all tested instances.

4 Conclusion

Three new exact algorithms were presented to calculate motifs using combinatorial techniques. The algorithms have complexity \( O(m^{\sqrt{m}}) \) to count isomorphic patterns of size 3 and \( O(m^2) \) to count isomorphic patterns of size 4 and \( O(m^2 n) \) to count isomorphic patterns of size 5. Computational results show that the proposed exact algorithms are expressively faster than the known techniques (e.g., FANMOD or Kavosh).

5 Availability and requirements

Project name: acc-Motif - Accelerated Motif Detection Using Combinatorial Techniques
Project home page: \url{http://www.ft.unicamp.br/~meira/accmotifs}
Operating system(s): Platform independent
Programming language: Java
Other requirements: e.g. Java 1.6. 1GB Ram.
License: Freeware.
Any restrictions to use by non-academics: None.

6 Authors’ contributions

All authors are involved in algorithms discussion and manuscript writing. L. A. A. Meira and V. R. Máximo are involved in the java implementation.
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8 Competing interests

The authors declare that they have no competing interests.

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\[ A^v = \delta^*(v) \]

\[ B^v = \delta^+(v) \]

\[ C^v = \delta^-(v) \]

\[ m_{a,b}^v = \delta^+(A^v, B^v) \]

\[ m_{a,c}^v = \delta^+(A^v, C^v) \]

\[ m_{b,c}^v = \delta^+(B^v, C^v) \]

\[ m_{a,a}^v = \delta^+(A^v, A^v) \]

\[ m_{b,b}^v = \delta^+(B^v, B^v) \]

\[ m_{c,c}^v = \delta^+(C^v, C^v) \]

\[ m_{a,b}^{\prime v} = \delta^*(A^v, B^v) \]

\[ m_{a,c}^{\prime v} = \delta^*(A^v, C^v) \]

\[ m_{b,c}^{\prime v} = \delta^*(B^v, C^v) \]

\[ m_{a,a}^{\prime v} = \delta^*(A^v, A^v) \]

\[ m_{b,b}^{\prime v} = \delta^*(B^v, B^v) \]

\[ m_{c,c}^{\prime v} = \delta^*(C^v, C^v) \]

Table 1: Variables to vertex v.

\[ \text{pattern}(\Delta, T_i, T_2) \quad \text{pattern}^+(\Delta, T_i, T_2) \quad \text{pattern}^-(\Delta, T_i, T_2) \quad \text{pattern}^{++}(\Delta, T_i, T_2) \]

Figure 8: Variations of matrix pattern(\Delta, T_i, T_j) for T_i = set(A, B, \emptyset) and T_j = set(\emptyset, \emptyset, C).
| Pattern | Frequency | Line |
|---------|-----------|------|
| $o \leftrightarrow o \rightarrow o$ | $n^v_a n^v_b - m^v_{a,b} - m^v_{b,a} - m^v_{a,b}$ | 1 |
| $o \leftrightarrow o \leftarrow o$ | $n^v_a n^v_c - m^v_{a,c} - m^v_{c,a} - m^v_{a,c}$ | 2 |
| $o \rightarrow o \rightarrow o$ | $n^v_b n^v_c - m^v_{b,c} - m^v_{c,b} - m^v_{b,c}$ | 3 |
| $o \leftrightarrow o \leftrightarrow o$ | $\left(\frac{n^v_a}{2}\right) - m^v_{a,a} - m^v_{a,a}$ | 4 |
| $o \leftarrow o \rightarrow o$ | $\left(\frac{n^v_b}{2}\right) - m^v_{b,b} - m^v_{b,b}$ | 5 |
| $o \rightarrow o \leftarrow o$ | $\left(\frac{n^v_c}{2}\right) - m^v_{c,c} - m^v_{c,c}$ | 6 |

Table 2: Isomorphic pattern frequencies involving vertex $v$ and two neighbors.

| Pattern | Frequency | Line |
|---------|-----------|------|
| $P_4$ | $n^v_x n^v_y - m^v_{x,y}$ | |
| $x \leftrightarrow C_3$ | $(n^e_x + n^e_y)n^e_z - m^e_{x,z} - m^e_{y,z} + m^e_{x,x} + m^e_{y,y}$ | |
| $S_3$ | $\left(\frac{n^e_x}{2}\right) + \left(\frac{n^e_y}{2}\right) - m^e_{x,x} - m^e_{y,y}$ | |
| $K_4 \setminus \{e\}$ | $\left(\frac{n^e_x}{2}\right) + m^e_{x,z} + m^e_{y,z} - m^e_{x,z}$ | |
| $C_4$ | $m^e_{x,y}$ | |
| $K_4$ | $m^e_{x,z}$ | |

Table 3: $e$-Patterns frequencies for $e = \{u, v\}$.

Table 4: If the top blue edge is ignored, this table represents pattern$(T_i, T_j)$ for all $T_i, T_j \in \mathcal{T}^e$. Symmetric side omitted.
| Pattern | Frequency |
|---------|-----------|
| ![Pattern](image1) | \(\binom{n_x}{2} + \binom{n_y}{2} + \binom{n_z}{2}\) |
| ![Pattern](image2) | \(n_{x_1}n_{x_2} + n_{x_1}n_{x_3} + n_{x_2}n_{x_3}\) |
| ![Pattern](image3) | \(n_{x_1}(n_{y_{12}} + n_{y_{13}}) + n_{x_2}(n_{y_{12}} + n_{y_{23}}) + n_{x_3}(n_{y_{13}} + n_{y_{23}})\) |
| ![Pattern](image4) | \(n_{x_1}n_{y_{23}} + n_{x_2}n_{y_{13}} + n_{x_3}n_{y_{23}}\) |
| ![Pattern](image5) | \((n_{x_1} + n_{x_2} + n_{x_3})n_{z}\) |
| ![Pattern](image6) | \(\binom{n_{y_{12}}}{2} + \binom{n_{y_{13}}}{2} + \binom{n_{y_{23}}}{2}\) |
| ![Pattern](image7) | \(n_{y_{12}}n_{y_{13}} + n_{y_{12}}n_{y_{23}} + n_{y_{13}}n_{y_{23}}\) |
| ![Pattern](image8) | \((n_{y_{12}} + n_{y_{13}} + n_{y_{23}})n_{z}\) |
| ![Pattern](image9) | \(\binom{n_{y}}{2}\) |

Table 5: \(K_3\)-Patterns frequencies for the graph of Figure 6. \(P_3\)-Patterns frequencies are analogous.
Pattern | Frequency | Line
--- | --- | ---
| \( \binom{n}{2} \) + \( \binom{n}{2} \) + \( \binom{n}{2} \) - \( m_{x_1,x_1} - m_{x_2,x_2} - m_{x_3,x_3} \) | 1 |
| \( n_x x_2 + n_x x_3 + n_x x_3 - m_{x_1,x_2} - m_{x_1,x_3} - m_{x_2,x_3} \) | 2 |
| \( n_x (n_{y_{12}} + n_{y_{13}}) + n_x (n_{y_{12}} + n_{y_{23}}) + n_x (n_{y_{13}} + n_{y_{23}}) - m_{x_1,y_{12}} - m_{x_1,y_{13}} - m_{x_2,y_{12}} - m_{x_2,y_{23}} - m_{x_3,y_{13}} - m_{x_3,y_{23}} \) | 3 |
| \( n_x n_{y_{23}} + n_x n_{y_{13}} + n_x n_{y_{23}} - m_{x_1,y_{23}} - m_{x_2,y_{13}} - m_{x_3,y_{12}} \) | 4 |
| \( (n_x + n_x + n_x) m_z - m_{x_1,z} - m_{x_2,z} - m_{x_3,z} \) | 5 |
| \( \binom{n_{y_{12}}}{2} + \binom{n_{y_{13}}}{2} + \binom{n_{y_{23}}}{2} - m_{y_{12},y_{13}} - m_{y_{12},y_{23}} - m_{y_{13},y_{23}} \) | 6 |
| \( n_{y_{12}} n_{y_{13}} + n_{y_{12}} n_{y_{23}} + n_{y_{13}} n_{y_{23}} - m_{y_{12},y_{13}} - m_{y_{12},y_{23}} - m_{y_{13},y_{23}} + m_{x_1,y_{12}} + m_{x_1,y_{13}} + m_{x_2,y_{12}} + m_{x_2,y_{23}} + m_{x_3,y_{13}} + m_{x_3,y_{23}} \) | 7 |
| \( (n_{y_{12}} + n_{y_{13}} + n_{y_{23}}) m_z - m_{y_{12},z} - m_{y_{13},z} - m_{y_{23},z} m_{x_1,z} + m_{x_2,z} + m_{x_3,z} + m_{y_{12},y_{13}} + m_{y_{12},y_{23}} + m_{y_{13},y_{23}} \) | 8 |
| \( m_{n_{y_{12}},n_{y_{13}}} + m_{n_{y_{12}},n_{y_{23}}} + m_{n_{y_{13}},n_{y_{23}}} \) | 9 |
| \( \binom{n}{2} \) - \( m_{zz} + m_{y_{12},z} + m_{y_{13},z} + m_{y_{23},z} \) | 10 |
| \( m_{x_1,x_1} + m_{x_2,x_2} + m_{x_3,x_3} \) | 11 |
| \( m_{x_1,x_2} + m_{x_1,x_3} + m_{x_2,x_3} \) | 12 |
| \( m_{x_1,y_{23}} + m_{x_2,y_{13}} + m_{x_3,y_{12}} \) | 13 |
| \( m_{z,z} \) | 14 |

Table 6: \( K_3 \)-Patterns frequencies in a general graph.
Table 7: $P_3$-Patterns frequencies in a general graph.
| Grafs      | (n,m)          | acc-Motif (ms) | Famod (ms)  | Kavosh (ms) |
|------------|----------------|---------------|-------------|-------------|
| E.coli     | (418, 519)     | 0.13 ± 0.005  | 8.0 ± 0.003 | 4.5 ± 0.02  |
| CSphd     | (1882, 1740)   | 0.68 ± 0.009  | 9.7 ± 0.001 | 5.3 ± 0.03  |
| Yeast      | (688, 1079)    | 0.25 ± 0.005  | 22.7 ± 0.03 | 11.5 ± 0.07 |
| Roget      | (1022, 5074)   | 2.1 ± 0.06    | 52.7 ± 0.01 | 30.2 ± 0.4  |
| Epa        | (4271, 8965)   | 4.4 ± 0.08    | 387.8 ± 0.1 | 202.4 ± 0.6 |
| California | (6175, 16150)  | 11.3 ± 0.14   | 632.4 ± 0.1 | 316.3 ± 0.5 |
| Facebook   | (1899, 20296)  | 14.2 ± 0.29   | 1,446 ± 0.6 | 576 ± 2     |
| ODLIS      | (2900, 18241)  | 18.0 ± 0.27   | 3,150 ± 2  | 957 ± 2     |
| PairsFSG   | (5018, 63608)  | 10.5 ± 6      | 3,883 ± 14 | 1,915 ± 3   |
| **Airport**| **(1574, 28236)** | **35 ± 0.2**  | **5,772 ± 2** | **1,250 ± 6** |
| Foldoc     | (12905, 109092)| 183 ± 0.3    | 7,481 ± 24 | 2,148 ± 5   |

Table 8: Execution time to count isomorphic patterns of size 3 by processed graph using acc-Motif, FANMOD and Kavosh.

| Grafs      | (n,m)          | acc-Motif (ms) | Famod (ms)  | Kavosh (ms) |
|------------|----------------|---------------|-------------|-------------|
| E.coli     | (418, 519)     | 3.7 ± 0.6     | 221.0 ± 0.2 | 124.0 ± 0.7 |
| CSphd     | (1882, 1740)   | 7.4 ± 0.2     | 104.5 ± 0.3 | 59.1 ± 0.5  |
| Yeast      | (688, 1079)    | 7.8 ± 0.1     | 573.7 ± 0.9 | 278.1 ± 0.8 |
| Roget      | (1022, 5074)   | 58 ± 1.3      | 930.8 ± 1.2 | 520.1 ± 2.1 |
| Epa        | (4271, 8965)   | 200 ± 7.4     | 26,613 ± 49 | 13,739 ± 15 |
| California | (6175, 16150)  | 772 ± 64      | 37,484 ± 101| 19,280 ± 110|
| Facebook   | (1899, 20296)  | 2135 ± 75     | 147,713 ± 169| 59,064 ± 277|
| **ODLIS**  | **(2900, 18241)** | **2,605 ± 115** | **630,936 ± 2,914** | **210,015 ± 837** |
| PairsFSG   | (5018, 63608)  | 9.097 ± 114   | 334,025 ± 454 | 181,957 ± 617|
| Airport    | (1574, 28236)  | 10,106 ± 130  | 794,227 ± 1091| 163,678 ± 1,065|
| Foldoc     | (12905, 109092)| 10,047 ± 30   | 1,179,759 ± 3,066 | 259,935 ± 690 |

Table 9: Execution time to count isomorphic patterns of size 4 by processed graph using acc-Motif, FANMOD and Kavosh.
| Grafos     | (n,m)             | acc-Motif (s) | FANMOD (s) | Kavosh (s) |
|-----------|-------------------|---------------|-------------|------------|
| E.coli 11 | (418,519)         | 0.1 ± 0.01    | 5.6 ± 0.02  | 3.5 ± 0.03 |
| CSphd 3   | (1882,1740)       | 0.1 ± 0.002   | 1.3 ± 0.03  | 0.76 ± 0.01|
| Yeast 1   | (688,1079)        | 0.3 ± 0.003   | 12.9 ± 0.07 | 7.5 ± 0.1  |
| Roget 5   | (1022,5074)       | 2 ± 0.005     | 17.4 ± 0.06 | 11.3 ± 0.07|
| Epa 3     | (4271,8965)       | 32.3 ± 0.1    | 1.696 ± 6   | 1.052 ± 5.9|
| California 3 | (6175,16150)   | 76 ± 0.4      | 2.376 ± 12  | 1.532 ± 12 |
| Facebook 20 | (1899,20296)    | 505 ± 6       | 14,378 ± 10 | 6,343 ± 25 |
| ODLIS 3   | (2900,18241)      | 835 ± 2.6     | > 13h       | > 13h      |
| PairsFSG 3 | (5018,63608)     | 2,334 ± 2.3   | > 13h       | 23,036.62 ± 23.6 |
| Airport 20 | (1574,28236)     | 3,058 ± 14    | > 13h       | 18,278.96 ± 37.66 |
| Foldoc 3  | (12905,109092)    | 2,965 ± 3.2   | > 13h       | > 13h      |

Table 10: Execution time to count isomorphic patterns of size 5 by processed graph using acc-Motif, FANMOD and Kavosh.