Fast Graphlet Transform of Sparse Graphs

Dimitris Floros*  Nikos Pitsianis*†  Xiaobai Sun†

*Department of Electrical and Computer Engineering
Aristotle University of Thessaloniki
Thessaloniki 54124, Greece
†Department of Computer Science
Duke University
Durham, NC 27708, USA

Abstract—We introduce the computational problem of graphlet transform of a sparse large graph. Graphlets are fundamental topology elements of all graphs/networks. They can be used as coding elements for encoding graph-topological information at multiple granularity levels on a graph, and for making differentiation and connection across different graphs and networks. Network/graph analysis using multiple graphlets has growing applications. We recognize the universality and increased encoding capacity in using multiple graphlets, we address the arising computational complexity issues, and we present a fast method for exact graphlet transform. The fast graphlet transform establishes a few remarkable records at once in high computational efficiency, low memory consumption, and ready translation to high-performance program and implementation. It is intended to facilitate or enable advanced network/graph analysis with graphlets, and to advance at the same time sparse graph theory, high-performance graph computation and broader applications.

Index Terms—network analysis, topological encoding, fast graphlet transform

I. INTRODUCTION

Network analysis using graphlets has advanced in recent years. The concepts of graphlets, graphlet frequency, and graphlet analysis are originally introduced in 2004 by Pržulj, Corneil and Jurisica [11]. They are substantially extended in several ways, [15], [18], [20]. Graphlets are mostly used for statistical characterization and modeling of entire networks. In the work by Palla et. al. [9], which is followed by many, a network of motifs (a special case of graphlets) is induced for overlapping community detection on the original network. Recently we established a new way of using graphlets for graph analysis. We use graphlets as coding elements to encode topological and statistical information of a graph at multiple granularity levels within a graph, from micro-scale structures at vertex neighborhoods, up to macro-scale structures such as cluster configurations [5]. We also use the topology encoded information to uncover temporal patterns of variation and persistence across networks in a time-shifted sequence, not necessarily over the same vertex set [6].

We anticipate a growing interest in, and applications of, graphlet-based network/graph analysis, for the following reasons. Graphlets are fundamental topology elements of all networks or graphs. See a particular graphlet dictionary shown in Fig. 1. Conceptually, graphlets for network/graph analysis are similar to wavelets for spectro-temporal analysis in signal processing [14], shapelets for time series classification [21], super-pixels for image analysis [13], and n-grams for natural language processing [16], [17]. Like motifs, graphlets are small graphs. By conventional definition, motifs are small subgraph patterns that appear presumptively and significantly more frequently in a network under study. Motif analysis relies on prior knowledge or assumption [7]. Graphlets are ubiquitous; graphlet analysis reveals the most frequent connection patterns or motifs, or lack of dominance by any, in a network.

There is another aspect of the universality in using graphlets. Graphlets are defined in the graph-topology space. They are not to be confused with the wavelets applied to the spectral elements of a particular graph Laplacian as in certain algebraic graph analysis. The latter is limited to the family of graphs defined on the same vertex set and share the same eigenvectors. Otherwise, the Laplacians of two graphs even defined on
the same vertex set are not commutable. The computation of Laplacian spectral vectors and values is also limited, by computational complexity and resource, to low dimensional invariance subspaces.

The time and space complexities of graph encoding with graphlets, i.e., the graphlet transform, have not been formally described and addressed. We formally describe the graphlet transform in Section II, with which we obtain the graphlet frequencies at all vertices on a network/graph. In fact, this is related to the classical problem of finding, classifying and counting small subgraphs over vertex neighborhoods [4], [12]. A familiar case is to find and count all triangles over the entire graph. The triangle is graphlet $\sigma_4$ ($C_3, K_3$) in the dictionary in Fig. 1. With the graphlet transform, we count in more detail – the number of distinct triangles incident on each and every vertex. We found from our recent analysis of scientific collaboration networks [6] that the bi-fork graphlet $\sigma_3$ ($K_{1,2}$) encodes the betweenness between triangle clusters. The bi-fork betweenness is to be calculated at each and every vertex. Another familiar case is to find and count induced subgraphs with the pattern of the claw graphlet $\sigma_8$ ($K_{1,3}$).

The time complexity for calculating the number of claws over all vertices of graph $G = (V, E)$ is $O(n^4)$, $n = |V|$, by the naive method that checks every connected quad-node subgraph to see if it is a claw. The naive method can be accelerated in asymptotic complexity by applying fast matrix multiplication algorithms on asymptotically sufficiently large graphs, at the expense of greater algorithmic complication, and if feasible to implement, with increased memory consumption, loss of data locality and increased latency in memory access on any modern computer with hierarchical memory. Due to the high complexity, some network analysis with graphlets resort to nondeterministic approximation with sparse sampling under a necessary structure-persistent assumption [12]. It is known otherwise that certain network properties are not preserved with sampling [19].

The present work makes a few key contributions. We formally introduce the graphlet transform problem, and address both the encoding capacity and the encoding complexity issues. We present the fast method for graphlet transform of any large, sparse graph, with any sub-dictionary of $\Sigma_{16}$ as the coding basis. The solution is deterministic, exact and directly applicable to any range of graph size. Our solution method establishes remarkable records at once in multiple aspects – time complexity, memory space complexity, and in data structure and program complexity for algorithm implementation. Particularly, for any dictionary $\Sigma$ composed of coding elements among the first 14 graphlets in Fig. 1, for a graph $G = (V, E)$ with bounded degree, the time and space complexities of our fast graphlet transform are linear in $|V| + |E|$. At the same time, the transform formulas can be straightforwardly translated to high performance computation, via the use of readily available software libraries such as GraphBLAS\(^1\). We address also the effect of a chosen dictionary (coding book) on computational complexities. Our objectives of developing the fast graphlet transform are twofold: to facilitate or enable the paradigm shift to graph analysis with graphlets and to enrich and advance sparse graph computation and its applications.

II. GRAPHLET TRANSFORM: PROBLEM DESCRIPTION

We now describe generic graphlets and graphlet dictionaries by their forms and attributes, with modification in description over the original for clarity. A graphlet is a connected graph with a small vertex set and a designated node to be incident with. We show in Fig. 1 a dictionary of 16 graphlets, $\Sigma = \Sigma_{16} = \{ \sigma_k \}_{k=0:15}$. The graphlets in the dictionary have the following patterns: singleton/vertex, edge ($K_2$), 2-path ($P_2$), binary fork ($K_{1,2}$), triangle ($C_3, K_3$), 3-path ($P_3$), binary fork ($K_{1,2}$), claw ($K_{1,3}$), dipper, 4-cycle ($C_4$), diamond, and tetrahedral ($K_4$). Each graphlet has a designated incidence node, which is shown with a red square, up to an isomorphic permutation (shown in red circles). Graphlets with the same number of nodes form a family with an internal partial ordering. For example, $\sigma_2, \sigma_3$ and $\sigma_4$ are a family of tri-node graphlets. The partial ordering $\sigma_2, \sigma_3 \prec \sigma_4$ is by the relationship that $\sigma_2$ and $\sigma_3$ are subgraphs of $\sigma_4$. Our rules for the ordering/labeling are described in the caption of Fig. 1 for convenience in visual verification.

Let $G = (V, E)$ be a graph. Let $\Sigma$ be a graphlet dictionary, the code book. We use a vertex-graphlet incidence structure to describe the process of encoding $G$ over the entire vertex set $V$ with coding elements in $\Sigma$. Denote by $B = (V; \Sigma; E_{\sigma})$ the bipartite between the graph vertices and the graphlets, $E_{\sigma} \subset V \times \Sigma$. There is a link $(v, \sigma)$ between a vertex $v \in V$ and a graphlet $\sigma \in \Sigma$ if $v$ is an incident node on a subgraph of $\sigma$-pattern. The incident node on a graphlet is uniquely specified, up to an isomorphic mapping. For example, graphlet $\sigma_6$ (clique $K_4$) in Fig. 1 is an automorphism. There may be multiple links between $v$ and $\sigma_k$. We denote them by a single link $(v, \sigma_k)$ with a positive integer weight $d_k(v)$ for the multiplicity, which is the frequency with graphlet $\sigma_k$. However, the multiplicities from vertex $v$ to multiple graphlets in the same family are not independently determined. For example, the multiplicities on links from vertices to $\sigma_2$ do not include those within $\sigma_4$. The weight on $(v, \sigma_1)$ is counted independently as $\sigma_1$ has no other family member. For any vertex, $d_0(v) = 1, d_1(v)$ is the ordinary degree of $v$ on graph $G$. With $k > 1$, $d_k(v)$ is a pseudo degree, depending on the internal structure of the family $\sigma_k$ is in. This vertex-graphlet incidence structure is a generalization of the ordinary vertex-edge incidence structure.

The graphlet transform of graph $G$ refers to the mapping $f$ of $G$ to the field of graphlet frequency vectors over $V$,

$$f(v) = [d_0(v), d_1(v), \ldots, d_K(v)]^T, \quad v \in V. \quad (1)$$

The vector field encodes, with graphlets as the encoding words/elements, the topological and statistical information of the graph. In the rest of the paper we introduce how we make the transform fast.

We consider first the coding capacity. The dictionary $\Sigma_2 = \{ \sigma_0, \sigma_1 \}$ is the minimal. It limits the network analysis to the

\(^1\)http://graphblas.org
ordinary degree distributions, types, correlations and models [1], [8], [10]. The dictionary $\Sigma_5$, a sub-dictionary of $\Sigma_{16}$, already offers much greater coding capacity. We address and answer an additional, interesting question – how the computation complexity changes with the choice of the coding elements.

III. FAST GRAPHLET TRANSFORM WITH $\Sigma_5$

A. Preliminary: graph of paths & graph of cycles

We start with path and cycle counting via graphs of paths and graphs of cycles, using matrix vector multiplications and additions. Denote by $G(P_\ell) = (V, E_\ell^P)$ the graph of length-$\ell$ paths over $V \times V$ with adjacency matrix $P_\ell$, $\ell > 0$. Element $P_\ell(i, j)$ is the number of length-$\ell$, simple (i.e., loop-less) paths between node $i$ and node $j$. Denote by $p_\ell$ the vertex function/vector, i.e., a scalar function defined on all vertices of $G$, such that $p_\ell(i)$ is the total number of length-$\ell$ paths that end at node $i$ from any other node. Then, $p_\ell(i) = \sum_j P_\ell(i, j)$.

In matrix-vector expression, $p_\ell = P_\ell \cdot e$, $\ell \geq 1$, (2)

where $e$ denotes the vector with all elements equal to 1. In particular,

$P_1 = A$, $p_1 = d_1$, $P_2 = A^2 - \text{diag}(d_1)$.

(3)

We use the convention that diag denotes the construction or extraction of a diagonal matrix, as used in MATLAB. Assume $G$ is degree bounded, $d_{1,\text{max}} = \|d_1\|_\infty$ is independent of $n = |V|$. Then,

$\text{nnz}(P_2) \leq d_{1,\text{max}} \cdot \text{nnz}(A) = O(|E|)$.

(4)

Denote by $G(C_\ell) = (V, E_\ell^C)$ the graph of length-$\ell$ cycles over $V \times V$ with adjacency matrix $C_\ell$, $\ell > 1$. Element $C_\ell(i, j)$ is the number of length-$\ell$ simple cycles that pass through both $i$ and $j$. Denote by $c_\ell$ the vertex function/vector, i.e., a scalar function defined on all vertices of $G$, such that $c_\ell(i)$ is the total number of length-$\ell$ simple cycles passing through node $i$. A simple cycle is a simple path that starts from and ends at the same node.

Denote by $\odot$ the Hadamard product, i.e., elementwise product. The following lemma states an important property of the graph of cycles.

Lemma 1 (Sparse graph of cycles). Let $G = (V, E)$ be a sparse graph with adjacency matrix $A$. For $\ell > 1$, a graph of $\ell$-cycles on $G$ can be expressed the sparse adjacency matrix $C_\ell$,

$C_\ell = A \odot P_{\ell-1}$.

(5)

Matrix $C_\ell$ is no denser than $A$. The vertex function $c_\ell$ is

$c_\ell = \frac{1}{\ell - 1} C_\ell \cdot e$.

(6)

In particular, $C_2 = A$, $c_2 = d_1$ and $C_3 = A \odot A^2$, $c_3 = C_3 \cdot e / 2$.

An immediate consequence of the cycle-sparse lemma is the fast formulation of $p_2$,

$p_2 = Ap_1 - c_2$.

(7)

It takes only one additional matrix-vector product with sparse matrix $A$.

B. Tri-node graphlet frequencies

There are 3 members in the tri-node graphlet family. Graphlet $\sigma_2$ is the 2-path, with the incidence node at an end. Graphlet $\sigma_3$ is the bi-ork, $K_{1,2}$, with the incidence node at the root. Graphlet $\sigma_4$ is the triangle, i.e., 3-cycle $C_3$ or 3-clique $K_3$. There is a partial ordering within the family,

$\sigma_2 \prec \sigma_3 \prec \sigma_4$

(8)

by the relationship that $\sigma_4$, the triangle, has $\sigma_2$ and $\sigma_3$ as subgraphs. The frequency with $\sigma_2$ at node $i$ in graph $G$ does not include those $\sigma_2$ subgraphs in any triangle. Similarly with the $\sigma_3$ frequency at any node.

Lemma 2 (Bi-fork graphlet frequencies). Let $G = (V, E)$ be an undirected graph. The bi-graphlet frequencies can be expressed in vector form as follows,

$d_3 = p_1 \odot (p_1 - 1)/2 - 2c_3$.

(9)

With $p_1$ and $c_3$ readily available, $d_3$ can be obtained with vector operations only.

Recall that we already have the vertex functions/vectors $d_0 = e$, $d_1 = A e$ and $d_4 = c_3$. It is straightforward to verify that $d_2 = p_2 - c_3$. Together, we have the following theorem.

Theorem 1 (Fast graphlet transform with $\Sigma_5$). The graphlet transform of $G$ with $\Sigma_5$ takes $\alpha \cdot d_{1,\text{max}}|E|$ arithmetic operations and $\beta(|E| + |V|)$ memory space, $\alpha < 3$ and $\beta < 6$.

IV. FAST GRAPHLET TRANSFORM WITH $\Sigma_{16}$

We turn our attention to the family of quad-node graphlets. The family has 11 members ($\sigma_5$ to $\sigma_{13}$) with the following partial ordering in terms of subgraph relationship,

$\sigma_5, \sigma_6 \prec \sigma_9, \sigma_{10}, \sigma_{11}, \sigma_{12}$;

$\sigma_7, \sigma_8 \prec \sigma_9, \sigma_{10}, \sigma_{11}$;

$\sigma_9, \sigma_{10}, \sigma_{11}, \sigma_{12} \prec \sigma_{13}, \sigma_{14}$;

$\sigma_{13}, \sigma_{14} \prec \sigma_{15}$.

(10)

With each graphlet $\sigma_i$ we derive first the formula for its raw frequency at vertex $v$, denoted by $d_i(v)$, as the number of $\sigma$-pattern subgraphs incident with $v$, including the induced ones. The raw frequency vector is $f(v) = (d_0(v), d_1(v), \ldots, d_{15}(v))^T$.

We will then convert the raw frequencies to the nested, or net, frequencies of (1). The net frequencies depend on the inter-relationships between the graphlets in a dictionary, as shown by the partial ordering in (10) for $\Sigma_{16}$. We always have $f(v) \geq f(v)$. When, and only when, the family of $k$-node graphlets is complete and non-redundant (no two family members are isomorphic), the net frequency at vertex $v$ is the number of $\sigma$-pattern induced subgraphs incident with $v$. 
For instance, a 3-star (claw) subgraph in a dipper is not the induced graph by the same vertex set. Under the complete and non-redundant family condition, the frequency conversion has the additional functionality to identify precisely the patterns of induced subgraphs. We will describe in Section V a unified scheme for converting raw frequencies to net ones. The condition on graphlet families can be relaxed for graph encoding purposes other than pattern recognition.

We derive fast frequency formulas for quad-node graphlets in 3 subgroups. Let $a$ and $b$ be non-negative vectors. We use $a - b$ as the shorthand expression for the rectified difference $\max\{a-b,0\}$ unless specified otherwise.

**A. The 3-paths & 4-cycle**

We relate the frequencies with 3-path graphlet $\sigma_5$ and gate graphlet $\sigma_6$ to that with $p_1$ and $p_2$. The following are straightforward.

$$d_5 = p_3, \quad d_6 = p_2 \circ (p_1 - 1) - 2c_3. \quad (11)$$

By the following lemma, we get the vector $p_3$ without constructing matrix $P_3$, which involves the cubic power of $A$.

**Lemma 3 (Fast calculation of 3-path frequencies).**

$$p_3 = A p_2 - p_1 \circ (p_1 - 1) - 2c_3. \quad (12)$$

**Proof.** We have $p_3 = P_3 e$, where

$$P_3 = A P_2 - \text{diag}(p_1 - 1) \cdot P_1 - 2 \text{diag}(c_3). \quad (13)$$

We extend $P_2$ by one more step with the first term, remove one-step backtrack in the second term on returning paths, and then remove triangles.

Next, we obtain the vector $c_4$ without constructing $C_4 = A \odot P_3$ via $P_4$ as by the inductive step of Lemma 1.

**Lemma 4 (Fast calculation of 4-cycle frequencies).** Denote by $G(C_{4,2})$ the graph with adjacency matrix $C_{4,2}$ such that element $C_{4,2}(i,j)$ is the number of distinct 4-cycles passing through node $i$ and node $j$ at diametrical positions. Then

$$C_{4,2} = P_2 \circ (P_2 - 1), \quad c_4 = C_{4,2} \cdot e/2, \quad (14a, 14b)$$

where the subtraction by 1 is taken at the nonzero elements only. Consequently, $C_{4,2}$ is no denser than $P_2$, $\text{nnz}(C_{4,2}) \leq \text{nnz}(P_2)$.

By the diametrical symmetry, $\sum_j C_{4,2}(i,j)$ is twice the total number of 4-cycles passing through $i$. Matrix $C_{4,2}$ may be much sparser than $P_2$, see (3).

The essence of our fast frequency calculation lies in constructing sparse auxiliary matrices in which Hadamard products are used to incorporate logical conditions and to multiply the frequency factors together. With this in mind, we present the frequency calculation for the remaining 8 graphlets with brief statements in comparison to the previous ones. We sketch a proof for a formula when necessary.

**B. The claws & dippers**

This section contains fast formulas for raw frequencies with two claw graphlets and three dipper graphlets. Graphlet $\sigma_7$ is the claw with the incidence node at a leaf node. At node $i$, we sum up the bi-fork counts over its $p_1$ neighbors, excluding the one connecting to $i$, i.e., $(p_1(i) - 1)$ choose 2. Thus,

$$d_7 = A \cdot ((p_1 - 1) \circ (p_1 - 2))/2. \quad (15)$$

Graphlet $\sigma_8$ is the claw $(K_{1,3})$ with the incidence node at the root/center. We have

$$d_8 = p_1 \circ (p_1 - 1) \circ (p_1 - 2)/3!, \quad (16)$$

by the fact that the number of 3-stars centered at a node $i$ is $p_1(i)$ choose 3.

Graphlet $\sigma_9$ is the dipper with the incidence node at the handle end. We have

$$d_9 = A \cdot c_3 - 2c_3. \quad (17)$$

The triangles passing $i$ are removed from the total number of triangles incident at the neighbor nodes of $i$.

Graphlet $\sigma_{10}$ is the dipper with the incidence node at a base node. We have

$$d_{10} = C_3 \cdot (p_1 - 2). \quad (18)$$

Each triangle at node $i$ is multiplied by the number of other adjacent nodes that are not on the same triangle. By Lemma 1, $C_3$ is as sparse as $A$.

Graphlet $\sigma_{11}$ is the dipper with the incidence node at the center (degree 3). We have

$$d_{11} = (p_1 - 2) \circ c_3. \quad (19)$$

At the incident node $i$, the number of triangles is multiplied by all other edges leaving node $i$.

For this group of graphlets, the calculation of the raw frequencies uses either vector operations or matrix-vector products with the matrix as $A$ itself or as sparse as $A$.

**C. The diamonds & the tetrahedral**

Graphlet $\sigma_{13}$ is the diamond with the incidence node at an off-cord node $i$. We have

$$D_3 \triangleq \text{diag}(a_j^T (C_3 - A) a_j, j=1:n), \quad (20)$$

where $a_j$ is the column $j$ of $A$. By Lemma 1, the kernel matrix $(C_3 - A)$ is as sparse as $A$.

**Proof.** Any two nodes among the neighbors of $i$, indicated by $A(:,i)$, should belong to at least 2 triangles in the diamond, i.e., $(C_3 - A) \neq 0$, and one of the remaining 2 nodes in the triangles must loop back to node $i$.

Graphlet $\sigma_{14}$ is the diamond with the incidence node at a cord node. We have

$$d_{14} = (A \odot C_{4,2}) \cdot e/2. \quad (21)$$

The Hadamard matrix product is as sparse as $A$, the factor matrix $C_{4,2}$ is defined in Lemma 4.
Proof. Node $i$ and any of its direct neighbor node $j$, i.e., $A(i,j) = 1$, must be on the diametrical nodes of a 4-cycle $C_{4,2}(i,j) \neq 0$.

Graphlet $\sigma_{16}$ is clique $K_4$. Define matrix $T$ as follows,

$$T \triangleq A \odot [q_j^TA q_j], \quad q_{ij} = a_i \odot a_j,$$

where $a_j$ is the column $j$ of $A$. Matrix $T$ is as sparse as $A$ is. We have

$$d_{15}(i) = T \cdot e/6.$$

Proof. For every edge $(i,j)$, i.e., $A(i,j) \neq 0$, the vector $q_{ij}$ gives the (intersection) set of common neighbors between node $i$ and node $j$. The intersection size is bounded, $mnz(q_{ij}) \le \min\{d_1(i), d_1(j)\}$. If $q_{ij}(k)q_{ij}(\ell)A(k,\ell) \neq 0$, then the subgraph at $\{i,j,k,\ell\}$ is a tetrahedral. Thus, the total number of distinct tetrahedrals incident with edge $(i,j)$ is

$$T(i,j) = \sum_{k>\ell} q_{ij}(k)q_{ij}(\ell)A(k,\ell)/3 = q_j^TA q_j/6.$$

V. A UNIFIED SCHEME FOR FREQUENCY CONVERSION

We summarize in Table 1 the formulas in matrix-vector form for fast calculation of the raw graphlet frequencies. The auxiliary vectors are $p_1$ and $c_j$, $1 \le j \le 4$, each of which is elaborated in sections III and IV. The auxiliary matrices $C_5$, $A \odot C_{4,2}$, $D_4$ and $T$ are as sparse as $A$.

We provide in Table 2 the (upper triangular) matrix $U_{16}$ of nonnegative coefficients for mapping net frequencies $d(v)$ to raw frequencies $\bar{d}(v)$. To save space, we omit the matrix for the inverse transformation. The conversion matrix, invariant across the vertices, is applied to each and every vertex. The conversion matrix for any sub-dictionary is by the corresponding sub-matrix of $U_{16}$ and its inverse. The conversion coefficients are determined by subgraph-isomorphisms among graphlets and automorphisms in each graphlet. The same conversion method is applicable to a larger dictionary. In any case, frequency conversion takes no more than $|\Sigma| \cdot (|\Sigma| - 1) \cdot |V|$ arithmetic operations in total.

We illustrate in Fig. 2 the graphlet transform with a small graph $G = (V,E)$ with six vertices and nine edges. With each graphlet $\sigma_j$, the vertex vector $d_i$ is calculated by the fast formulas in Table 1, and tabulated in the top table/counts computed by our fast transforms. The $i$-th row in the table is then the raw frequency vector $\bar{f}(v_i)$. The raw frequency vectors $\{\bar{f}(v), v \in V\}$ are then converted to the net frequency vectors $\{f(v), v \in V\}$ of (1) by matrix-vector multiplications with the same triangular matrix $U_{16}$. The fast graphlet transform is exact. We made accuracy comparison between the results by our fast formulas and that by the dense counterparts. The results reach full agreement. What more meaningful and valuable is that the transform effectively enables systematic and economic quantification and recognition of topological properties of the graph, as briefly noted in the caption of Fig. 2.

VI. HIGH-PERFORMANCE GRAPHLET TRANSFORM

We address the high-performance aspect of graphlet transform. Our fast formulas are in ready form to be translated to high-performance program and implementation. All operations for the fast graphlet transform are products of sparse matrices, Hadamard products of matrices (which were rarely used in conventional graph counting methods) and products of sparse matrix with dense or sparse vectors.

As mentioned in Section IV-A, a distinguished and advantageous feature of our fast transform scheme is to design auxiliary matrices, in each of which we use the Hadamard product for both functions – to incorporate logical conditions and to multiply the factor counts together. Conventional counting schemes often resort only to the ordinary matrix multiplications and additions. In comparison, a lot of detours incur in traversing a graph. Conventional approaches become even more complicated by reducing time complexity with fast, recursive matrix multiplications, which are incapable of preserving sparsity and difficult to have perceivable efficiency.

| $\Sigma_{16}$ | Graphlet, incidence node | Formula in vector expression |
|--------------|--------------------------|-----------------------------|
| $\sigma_0$   | singleton                 | $a_0 = e$                   |
| $\sigma_1$   | 1-path, at an end         | $d_1 = p_1$                 |
| $\sigma_2$   | 2-path, at an end         | $d_2 = p_2$                 |
| $\sigma_3$   | bi-fork, at the root      | $d_3 = p_1 \odot (p_1 - 1)/2$|
| $\sigma_4$   | 3-clique, at any node     | $d_4 = c_3$                 |
| $\sigma_5$   | 3-path, at an end         | $d_5 = p_3$                 |
| $\sigma_6$   | 3-path, at an interior node | $d_6 = p_2 \odot (p_1 - 1) - 2c_3$|
| $\sigma_7$   | claw, at a leaf           | $d_7 = A \cdot ((p_1 - 1) \odot (p_1 - 2))/2$|
| $\sigma_8$   | claw, at the root         | $d_8 = p_1 \odot (p_1 - 1) \odot (p_1 - 2)/6$|
| $\sigma_9$   | dipper, at the handle tip | $d_9 = A \cdot c_3 - 2c_3$  |
| $\sigma_{10}$ | dipper, at a base node    | $d_{10} = c_3 \cdot (p_1 - 2)$|
| $\sigma_{11}$ | dipper, at the center     | $d_{11} = (p_1 - 2) \odot c_3$|
| $\sigma_{12}$ | 4-cycle, at any node      | $d_{12} = c_3$              |
| $\sigma_{13}$ | diamond, at an off-cord node | $d_{13} = D_4 \cdot e/2$  |
| $\sigma_{14}$ | diamond, at an on-cord node | $d_{14} = (A \odot C_{4,2}) \cdot e/2$|
| $\sigma_{15}$ | 4-clique, at any node     | $d_{15} = T \cdot e/6$       |

TABLE 2: The matrix $U_{16}$ for conversion from net frequencies to raw frequencies, $U_{16}f = f$, associated with dictionary $\Sigma_{16}$. The raw-to-net frequency conversion $f = U_{16}^{-1}f$ is used in the fast transform. All coefficients of $U_{16}$ are non-negative. A sub-dictionary with index set $s$ has the conversion matrix $U_{16}(s,s)$, $\{0,1\} \subseteq s \subseteq \{0,1,\ldots,15\}$. |
gain on networks of practically finite size. Our approach is straightforward and efficient by directly exploiting the sparsity.

A particular reoccurring pattern among the formulas is the matrix-vector product with the matrix as a Hadamard product of two matrices, \((A \otimes B)v\), with matrix \(A\) as (or as sparse as) the adjacency matrix for the sparse graph under consideration. The product is as sparse as \(A\), regardless how dense \(B\) is. Consider two particular matrices, \(C_3\) of Lemma 1 and \(T\) of (22). Each is defined as a Hadamard product of the adjacency matrix \(A\) and a denser factor (\(A^2\) or \(q_{ij} A q_{ij}\)). We utilize GraphBLAS and its native functionality of “masked” operations, where the output is computed/modified only where the mask elements are on, not off. Here, the adjacency matrix \(A\) serves also as the sparsity mask for the operations.

We get additional benefits in sparse storage and parallel graphlet transform with the use of GraphBLAS, which encapsulates high-performance sparse graph operations on modern computer architectures, especially on multi-core computers [2], [3]. The compressed sparse row (CSR) storage format is used internally by GraphBLAS. It facilitates efficient parallel computation, free of write conflicts.

VII. MAIN THEOREM & BEYOND

By the preceding analysis we have the following theorem.

**Theorem 2 (Fast graphlet transform with \(\Sigma_{16}\)).** The fast graphlet transform of graph \(G = (V, E)\) with dictionary \(\Sigma_{16}\), by the formulas in Table 1 and the frequency conversion scheme in Section V, has the following properties.

1) With any sub-dictionary \(\Sigma\) composed of graphlets from the first 14 elements of \(\Sigma_{16}\), the time complexity is \(O(d_{1,\text{max}} |V| E + |\Sigma|^2 |V|)\), with \(d_{1,\text{max}} = \|d_1\|_{\infty}\) and \(\alpha < 10\).

2) With dictionary \(\Sigma_{16}\), the time complexity is \(16(\beta d_{1,\text{max}}^2 |E| + 16|V|)\), \(\beta < 5\).

3) The space complexity for each case is \(\gamma (|V| + |E|)\), \(\gamma < 6\).

To our knowledge, the fast graphlet transform establishes a few remarkable records. The complexity analysis is directly applicable to graphs of any size, especially in practical range, without resorting to asymptotically large size. The analysis suggests that our fast method makes exact graphlet transform affordable and attractive for network analysis with graphlets. The analysis can be straightforwardly applied to more specific conditions. For example, the time complexity on graphs with bounded degree is linear with \(|E| + |V|\). If \(d_{1,\text{max}} = O(|E|^{1/4})\), we can recognize in \(O(|E|^{1.5})\) operations whether or not the graph is claw-free.

The statements in the main theorem are on time and space complexities, with the dictionary size as a simple factor. A larger dictionary offers an exponentially increased encoding capacity at only linearly increased computation cost. We shall also point out the other aspect of dictionary selection. Depending on the object of graphlet encoding, certain graphlets must be included in the dictionary together. For example, when we use the bi-fork \(\sigma_3\) to encode the betweenness among triangle clusters, the triangle graphlet \(\sigma_3\) must be included. For another example, for claw-free recognition or claw detection, it is necessary to include in the dictionary all the graphlets that have 3-stars as subgraphs.

The fast graphlet transform is presented with the intention not only to enable advanced network/graph analysis with graphlets, but also advance graph theory, high-performance graph computation and broaden their applications. We have illustrated in section V an untapped potential with graphlet transform for systematic classification of vertices and recognition of topological properties of a network/graph (not limited to statistical categorization of networks or graphs).
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