Estimation of Graphlet Counts in Massive Networks

Ryan A. Rossi, Rong Zhou, and Nesreen K. Ahmed

***Abstract*— Graphlets are induced subgraphs of a large network and are important for understanding and modeling complex networks. Despite their practical importance, graphlets have been severely limited to applications and domains with relatively small graphs. Most previous work has focused on *exact algorithms*; however, it is often too expensive to compute graphlets exactly in massive networks with billions of edges, and finding an approximate count is usually sufficient for many applications. In this paper, we propose an *unbiased graphlet estimation framework* that is: (a) fast with large speedups compared to the state of the art; (b) parallel with nearly linear speedups; (c) accurate with less than 1% relative error; (d) scalable and space efficient for massive networks with billions of edges; and (e) effective for a variety of real-world settings as well as estimating global and local graphlet statistics (e.g., counts). On 300 networks from 20 domains, we obtain <1% relative error for all graphlets. This is vastly more accurate than the existing methods while using less data. Moreover, it takes a few seconds on billion edge graphs (as opposed to days/weeks). These are by far the largest graphlet computations to date.**

***Index Terms*— Graphlets, network motifs, induced subgraphs, estimation methods, unbiased graphlet estimation, local graphlet count estimation, graphlet statistics, parallel algorithms, higher-order network analysis, machine learning.**

I. Introduction

GRAPHLETS are small *induced subgraphs*[1] and are important for many predictive and descriptive modeling and learning systems/tasks [1]–[8] such as image processing and computer vision learning systems that use neural networks [1], [9], network alignment [6], [10]–[12], classification [2], [3], visualization and sensemaking [13], [14], dynamic network analysis [15], [16], community detection [17]–[19], role discovery [20], anomaly detection [21], [22], and link prediction [8], [23], [24]. Unfortunately, the application and general use of graphlets (especially those of size $k = 4$ nodes and larger) remain severely limited to networks that are small enough to avoid the scalability and performance limitations of *exact* algorithms [13], [25]–[28]. For instance, Shervashidze *et al.* [3] take hours to count graphlets on small networks (i.e., a few hundreds/thousands of nodes/edges) for the graph classification [2].

In many applications, finding an "approximate" answer is usually sufficient where the exact answer is not worth the extra cost and time. The recent rise of big data [29] has made approximation methods even more critical [30], especially for practical applications [31]–[35]. More recently, the approximation methods have been proposed for important problems such as triangle counting [36]–[40], the shortest path problems [33], [41], finding max cliques [42], and many others.

This paper aims to overcome the above-mentioned computational limitations to make graphlets more accessible to other applications/domains with much larger graphs. In particular, this paper proposes a general graphlet estimation framework for deriving unbiased estimates[2] of a variety of graphlet statistics (e.g., frequency of an arbitrary k-vertex-induced subgraph) from a small set of edge-induced neighborhoods. The graphlet estimators provide accurate and fast approximations of a variety of global and local graphlet properties.[3] Intuitively, a global graphlet property assigns a single value (or distribution/map) to a graph G, whereas a local graphlet property assigns a single value (or distribution/map) to a particular graph element such as an edge or node of G [43]. An example of a global graphlet statistic is the total number of 4-cliques in G, whereas an example of a local statistic is the number of 4-cliques containing a certain graph element such as an edge or node.[4] Furthermore, a number of important machine learning tasks are likely to benefit from the proposed graphlet estimation framework, including graph anomaly detection [21], [22], entity resolution [44], role discovery [45], and relational classification [46].

The key contributions of this paper are as follows.

- **Graphlet estimation framework:** A general unbiased estimation framework is proposed for approximating global and local graphlet properties (such as counts) in massive networks with billions of edges. The framework is shown to be accurate, fast, and scalable for *both* dense and sparse networks of arbitrary size.
- **Accurate:** For all graphlets and data (300 graphs from 20 domains), the methods are more accurate than the existing state-of-the-art methods (<1% relative error) while using only a small fraction of the data. Provable error bounds are also derived and shown to be tight (see Section IV-B).
- **Efficient:** The proposed estimation algorithms are orders of magnitude faster than the recent state-of-the-art algorithm and take a few seconds as opposed to days/months.

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[1]The terms graphlet and induced subgraph are interchangeable.

[2]A graphlet estimate X_i is unbiased if $\mathbb{E}[X_i] = Y$ [36] and Y is the actual.

[3]The term *graphlet properties* is used more generally toer to graphlet (single-valued) statistics and distributions.

[4]Note that the total number of 4-cliques in G is an example of a global graphlet statistic since it is computed over all graph elements (edges and nodes) in G, as opposed to an individual graph element in G.

- **Parallel methods:** This paper proposes parallel graphlet estimation methods for shared and distributed memory architectures. Strong scaling results with nearly linear speedups are observed across a variety of networks.
- **Estimation of graphlet statistics—beyond counts:** This paper proposes estimation methods for both global and local graphlet counts, as well as other graphlet properties beyond simple counts (see Section II-B). This is in contrast to the existing estimation methods for graphlets [47]–[49] that focus only on approximating global graphlet counts.
- **Largest investigation and graphlet computations:** To the best of our knowledge, this paper provides: (i) the largest graphlet computations to date and (ii) the largest empirical investigation using 300+ networks from 20+ domains.

II. Localized Graphlet Estimation Framework

In this section, we propose a new family of graphlet estimation methods based on selecting a set of localized neighborhoods. This gives rise to the *localized graphlet estimation framework* (LGE) that serves as a basis for deriving unbiased and consistent estimators that are fast, accurate, and scalable for massive networks. As shown later in Section IV, LGE has many interchangeable components and is effective for a wide variety of networks, applications, and domains (e.g., biological, social, and infrastructure/physical networks), which have fundamentally different structural properties.

A. Preliminaries

Let $G = (V, E)$ be an undirected simple graph with $N = |V|$ vertices and $M = |E|$ edges. Sets are *ordered*, unless otherwise mentioned. Given a vertex $v \in V$, let $\Gamma(v) = \{w \,|\, (v, w) \in E\}$ be the set of vertices adjacent to v in G. Similarly, given an edge $e = (u, v) \in E$, let $\Gamma(e)$ denotes the edge neighborhood of e defined as

$$\Gamma(e) = \Gamma(u, v) = \Gamma(u) \cup \Gamma(v) \setminus \{u, v\} \tag{1}$$

where $\Gamma(u)$ and $\Gamma(v)$ are the neighbors of u and v, respectively. The (explicit) edge neighborhood is $\mathbf{\Gamma}_e = G(\{\Gamma(v) - u\} \cup \{\Gamma(u) - v\})$. The subgraph $\mathbf{\Gamma}_e$ consists of the set of vertices adjacent to v or u (noninclusive) and all edges between that set. Moreover, the degree of a vertex v denoted as $d_v = |\Gamma(v)|$ is equal to the number of edges that contain v. We also denote $\Delta(G)$ as the maximum vertex degree.

Definition 1 (Graphlet): *A graphlet $G_i = (V_k, E_k)$ is a connected-iuced subgraph consisting of a subset $V_k \subset V$ of k vertices from $G = (V, E)$ together with all edges whose endpoints are both in this subset $E_k = \{\forall e \in E \,|\, e = (u, v) \wedge u, v \in V_k\}$. By definition, a graphlet has one connected component.*

A k-graphlet is defined as an *induced subgraph* with k-vertices. Furthermore, we define $\mathcal{G}^{(k)}$ as the set of k-vertex-induced subgraphs and $\mathcal{G} = \mathcal{G}^{(2)} \cup \cdots \cup \mathcal{G}^{(k)}$. A graphlet frequency distribution (GFD) is defined in the following.

Definition 2 (Graphlet Frequency Distribution): *Given a graph (or graph elements such as an edge, node, or subgraph), the* GFD *is defined as $f_i = (X_i / \sum_i X_i)$ for all $i = 1, \ldots, |\mathcal{G}|$ where X_i is the frequency of graphlet G_i. The resulting vector $\mathbf{f} = [\cdots \; f_i \; \cdots]$ is the* GFD.

TABLE I
Summary of Graphlet Properties and Notation

Summary of the notation and properties for graphlets of size $k = \{2, 3, 4\}$. Note that ρ denotes density; Δ and $\bar{d}$ denote the max and mean degree; r denotes assortativity; $|T|$ is the total number of triangles in G.

		Description	ρ	Δ	$\bar{\mathrm{d}}$	r	$\lvert T\rvert$
	G_1	edge	1.00	1	1.0	1.00	0
	G_2	triangle	1.00	2	2.0	1.00	1
	G_3	2-star	0.67	2	1.33	-1.00	0
	G_4	4-clique	1.00	3	3.0	1.00	4
	G_5	chordal-cycle	0.83	3	2.5	-0.66	2
	G_6	tailed-triangle	0.67	3	2.0	-0.71	1
	G_7	4-cycle	0.67	2	2.0	1.00	0
	G_8	3-star	0.50	3	1.5	-1.00	0
	G_9	4-path	0.50	2	1.5	-0.50	0

A summary of the graphlet notation and important properties are provided in Table I.

B. Problem Formulation

The goal of this paper is to obtain fast and accurate estimates of a variety of graphlet statistics (e.g., counts). In particular, we focus on four basic types of graphlet statistics that can be described by two pairs of exclusive attributes: single-valued versus distribution and global versus local (See [43] for further details). Intuitively, the four types of graphlet properties are as follows.

- **P1** *Global single-valued statistics* such as the total number of 4-cycles in G.
- **P2** *Global distributions*, e.g., a GFD computed using the total graphlet frequencies of G.
- **P3** *Local single-valued statistics*, e.g., the number of 4-cycles containing a specific graph element such as an edge (node).
- **P4** *Local distributions*, e.g., a GFD of an individual graph element such as an edge (or node).

The proposed framework gives rise to the graphlet estimation methods that are fast and accurate for a variety of these four types of graphlet properties. Obviously, estimation methods for global/local graphlet *statistics* return a single value (scalar value), whereas the methods for global/local distributions return the estimated distribution.

Now, we define the specific graphlet statistics and distributions (from the above-mentioned four types of graphlet properties) that are estimated in this paper including:

- Counts of graphlets $G_i \in \mathcal{G}$, for all $i = 1, 2, \ldots |\mathcal{G}|$ or the count of a specific graphlet $G_i \in \mathcal{G}$. In particular, this paper proposes estimators for both global $\mathbf{X}_G = \begin{bmatrix} X_1 & X_2 & \cdots \end{bmatrix}$ and local graphlet counts $\mathbf{x}_i = \begin{bmatrix} x_1 & x_2 & \cdots \end{bmatrix}$ for edge $e_i \in E$.
- Graphlet frequency distributions (Definition 2).
- Aggregate (single valued) statistics such as the max, mean, median, variance, etc. These aggregate

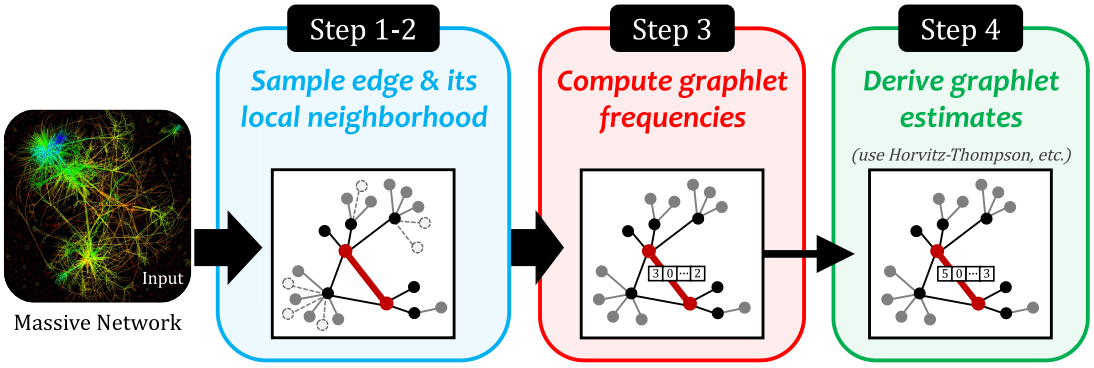


Fig. 1. Overview of the LGE framework for estimating local graphlet counts. The sampled edge from step 1 is shown in **red** (—) and highlighted. Unsampled neighbors shown in step 1–2 are dashed and light gray.

statistics are derived by calculating, choosing, or constructing a single value from a local statistic or distribution.

Estimators are derived for each of the above-mentioned graphlet problems. Existing estimation methods such as in [47]–[49] are limited to simple count statistics, whereas this paper instead proposes a unifying unbiased estimation framework that generalizes for a variety of other important graphlet properties beyond simple counts.[5] In addition, the previous work has mainly focused on estimating *global statistics* (e.g., total count of a graphlet in G), whereas this paper introduces estimators for both global *and* local graphlet statistics and distributions.

C. Framework Outline and Intuition

An overview of the LGE framework is provided in Fig. 1 for intuition. The LGE framework is based on the following general steps.

- **S1** Sampling a graph element (edge and node).
- **S2** Obtaining a localized subgraph H by sampling the local neighborhood (egonet) of that graph element.
- **S3** Given H, compute the graphlets containing the graph element (sampled from step **S1**).
- **S4** Use these counts to derive unbiased estimates (e.g., using the Horvitz–Thompson construction [36], [50]). Note that if we are estimating global graphlet statistics, then steps **S1**–**S3** are repeated K times prior to deriving estimates.

In this paper, we sample edge neighborhoods (as opposed to node neighborhoods). In particular, an edge neighborhood $\Gamma(e)$ is sampled with some probability from the set of all edge-induced neighborhoods (see Algorithm 1). Using the (potentially partial) edge neighborhood $\Gamma(e)$ centered at $e \in E$ as a basis, we compute the frequency of each graphlet $G_i \in \mathcal{G}$, for $i = 1, \ldots, |\mathcal{G}|$. Let us note that the edge (or node) may be selected uniformly at random or by an arbitrary weighted distribution $\mathbb{F}$ (as shown in Algorithm 1). The weighted distribution could be based on degrees, k-core numbers, or any attribute of interest. Furthermore, an edge (or node) neighborhood may be selected with a replacement or without. Selecting an edge neighborhood with replacement allows each edge neighborhood $\Gamma(e)$ to be used multiple times, whereas sampling without replacement ensures that each edge neighborhood included in the sample is unique (by label) and never repeated. Edge-centric graphlet decomposition algorithms[6] also lend themselves for (parallel) implementation on both shared memory and distributed memory architectures (see Section III). In addition, the fastest state-of-the-art subgraph counting approach can always be used in the proposed framework (see Step 3 in Fig. 1) to speedup the estimation even further. For instance, instead of using PGD [13] to count graphlets (as done in this paper), one can always use the fastest state-of-the-art subgraph counting algorithm.

A taxonomy for graphlet estimation is proposed in Table II. In particular, the existing graphlet estimation methods can be categorized as *direct graphlet estimation methods* since they sample a set of k-vertices *directly* from G and retrieve the k-graphlet induced by that set, whereas the proposed class of LGE methods select an edge and sample locally from the neighborhood. Table II also summarizes the existing estimation methods as well as our proposed approach according to the global and local graphlet (single valued) statistics and distributions estimated by each, as well as computational and algorithmic properties offered by each approach. Section II-D introduces a general estimation framework for global graphlet statistics, whereas Section II-E proposes a framework for estimating local graphlet statistics.

D. Estimation of Global Graphlet Statistics

Given the sampled set of edge-centric neighborhood, we show how to compute the estimated graphlet counts in Algorithm 2. More formally, let $T_e = \Gamma(u) \cap \Gamma(v)$ be the set of nodes that complete triangles with $e(v, u) \in J$. Likewise, $S_u = \{w \in \Gamma(u) \setminus \{v\} | w \notin \Gamma(v)\}$ and $S_v = \{w \in \Gamma(v) \setminus \{u\} | w \notin \Gamma(u)\}$, and thus $|S_v|$ and $|S_u|$ are the number of 2-stars centered at v and u, respectively. These quantities are computed in Lines 5–9 of Algorithm 2. For further intuition, see Fig. 2. Let us also note that $\Psi(\cdot)$ is a hash table for checking

[5] As an aside, counts have been used for many important measures in computational biology such as the graphlet degree distribution [11] and agreements [11].

[6] The term edge-centricers to algorithms that iterate over edges as opposed to nodes, see [51].

TABLE II
COMPARISON OF GRAPHLET ESTIMATION METHODS

Qualitative and quantitative comparison of the two main classes of graphlet estimation methods, namely, *direct methods* are those that sample k-vertices directly and retrieve the graphlet induced by that subset, whereas the proposed family of *localized graphlet estimation* (LGE) methods select ℓ-neighborhoods for estimation (and sample from them). The first six columns refer to the *global* and *local* graphlet estimation problems. In particular, columns 1-3 refer to the *global* graphlet statistics and distributions estimated by the methods (counts, GFD, and others such as extremal statistics/distributions, etc.), whereas columns 4-6 refer to the *local* graphlet statistics and distributions. "Parallel" refers to parallel estimation methods. "Space efficient" holds true if the space requirements of the algorithm are sublinear (preferably poly-logarithmic in the size of the input). "Streaming" holds true if the method is amenable to streaming implementation. "Position-aware" is true if the algorithm supports position-aware graphlets (orbits). "Sparse & dense" is true if the method has limited assumptions, and designed/capable of handling both sparse and dense graphs. "Parameter-free" methods are those that do not expect any user-specified input parameters (though they can be set, but is not required). "All graphlets" holds true if the method computes graphlet statistics and distributions for all graphlets up to size k.

		Global			Local			Computational						
	Method	**Counts**	**GFD**	**Others**	**Counts**	**GFD**	**Others**	**Parallel**	**Space efficient**	**Streaming**	**Position-aware**	**Sparse & dense**	**Parameter-free**	**All graphlets**
DIRECT	SHERV. *et al.* [3]		✓						✓	✓				
	GUISE [47]		✓											
	GRAFT [48]		✓											
	3-PATH SAMP. [49]	✓												
LGE	UNIFORM	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
	KCORE	✓	✓	✓	✓	✓	✓	✓			✓		✓	✓

edge existence in $o(1)$ time (see Algorithm 2). As an aside, this is an implementation detail and $\mathbf{\Psi}(\cdot)$ can easily be replaced with another data structure (bloom filters) or even removed entirely in favor of binary search (which may be favorable in situations where memory is limited). These possibilities are discussed in detail later. Note that $\mathbf{\Psi}(\cdot)$ is also used as a way to encode the different types of nodes. Thus, nodes are hashed using λ_1, λ_2, and λ_3, which may be defined as any unique symbol. In our implementation, we avoid the cost of resetting by ensuring that each λ_i is unique for each edge-centric neighborhood. In Line 4 of Algorithm 2, we mark the neighbors $\Gamma(v)$ of v as λ_1. Later in Line 8, a triangle is marked with λ_3, whereas Line 9 encodes a wedge as λ_2.

Next, Algorithm 2 maintains the *unrestricted graphlet counts*[7] in the following equations:

$$C_5 \pm \binom{|T_e|}{2} \tag{2}$$

$$C_6 \pm |T_e| \cdot (|S_u| + |S_v|) \tag{3}$$

$$C_8 \pm \binom{|S_u|}{2} + \binom{|S_v|}{2} \tag{4}$$

$$C_9 \pm |S_u| \cdot |S_v| \tag{5}$$

The quantities C_5, C_6, C_8, and C_9 are later used to derive chordal cycles, tailed triangles, 3-stars, and 4-paths in $o(1)$ time, respectively. In addition, we maintain C_2, C_3, C_4, and C_7 (see Algorithm 2). These quantities are computed for each edge-centric neighborhood in the sample, and then used for estimation. In particular, the three-vertex graphlet counts are estimated as follows:

$$X_2 = W_2 \sigma_2 C_2 \tag{6}$$

$$X_3 = W_3 \sigma_3 C_3 \tag{7}$$

where X_2 and X_3 are the estimated counts of graphlets G_2 and G_3, respectively. Similarly, the 4-vertex graphlet counts are estimated through the following equations:

$$X_4 = W_4 \sigma_4 C_4 \tag{8}$$

$$X_5 = W_5 \sigma_5 (C_5 - C_4) \tag{9}$$

$$X_6 = W_6 (\sigma_6 C_6 - 4 X_5) \tag{10}$$

$$X_7 = W_7 \sigma_7 C_7 \tag{11}$$

$$X_8 = W_8 (\sigma_8 C_8 - X_6) \tag{12}$$

$$X_9 = W_9 \sigma_9 (C_9 - C_7) \tag{13}$$

where X_4–X_9 are the estimated counts of the graphlets G_4–G_9, respectively. Furthermore, $\mathbf{W} \in \mathbb{R}^\kappa$ is a weight vector to account for the edge multiplicities

$$\mathbf{W} = \begin{bmatrix} 1 & \frac{1}{3} & \frac{1}{2} & \frac{1}{6} & 1 & \frac{1}{2} & \frac{1}{4} & \frac{1}{3} & 1 \end{bmatrix}^T \tag{14}$$

Algorithm 1 LGE framework for estimating *global graphlet statistics*

Input:
a graph $G = (V, E)$
a sample size K, or sample probability p
1: **parallel for** $j = 1, 2, \ldots, K$ **do**
2: Select e via an arbitrary (weighted/uniform) distribution $\mathbb{F}$
3: Set $J \leftarrow J \cup \{e\}$
4: Obtain estimated graphlet counts $\mathbf{X}$ for J via Alg. 2
5: **return** $\mathbf{X}$ – the estimated graphlet counts

Algorithm 2 Family of parallel LGE methods for deriving unbiased estimates of *global graphlet statistics*

Input: a graph G and a set of sampled edges J
1: **parallel for each** $e = (v, u) \in J$ in order **do**
2: Reset $T_e = \emptyset$ and $S_u = \emptyset$
3: **for** $w \in \Gamma(v)$ **do**
4: **if** $w \neq u$ **then** $\mathbf{\Psi}(w) = \lambda_1$
5: **for** $w \in \Gamma(u)$ **do**
6: **if** $w = v$ **then continue**
7: **if** $\mathbf{\Psi}(w) = \lambda_1$ **then**
8: $T_e \leftarrow T_e \cup \{w\}$ and set $\mathbf{\Psi}(w) = \lambda_3$ ▷ triangle
9: **else** $S_u \leftarrow S_u \cup \{w\}$ and set $\mathbf{\Psi}(w) = \lambda_2$ ▷ wedge
10: Update unrestricted counts via Eq. 2–5
11: $C_2 \pm |T_e|$ ▷ Note $\pm$ is the addition sum $C_2 = C_2 + |T_e|$
12: $C_3 \pm C_3(e) = (d_u + d_v - 2) - 2|T_e|$ ▷ equiv. $|S_u| + |S_u|$
13: $C_4 \pm C_4(e) = \text{CLIQUE}(\mathbf{\Psi}, T_e)$ ▷ in parallel (Alg. 3)
14: $C_7 \pm C_7(e) = \text{CYCLE}(\mathbf{\Psi}, S_u)$ ▷ in parallel (Alg. 4)
15: **end parallel**
16: Compute estimated graphlet counts $\mathbf{X}$ via Eq. 6-13
17: **return** $\mathbf{X}$, where X_i is the estimate for graphlet G_i

where each W_i is used to correct the counts of graphlet G_i [13]. Furthermore, we also define $\mathbf{p} \in \mathbb{R}^\kappa$ as a vector of sampling probabilities where p_i is the sampling probability for graphlet $G_i \in \mathcal{G}$. Note that p_i can be proportional to

[7]Note all count variables are initialized to zero; and $\pm$ is the addition assignment operator.

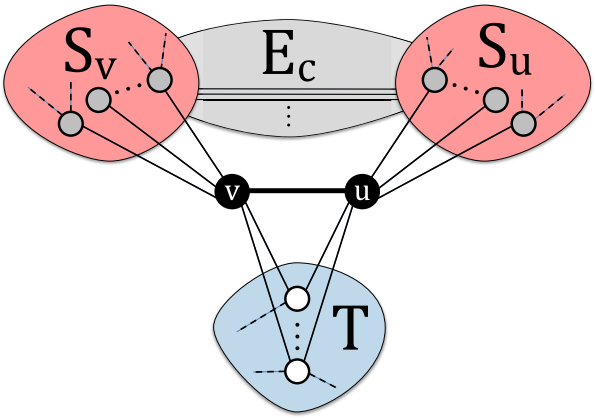


Fig. 2. Let T be the set of nodes completing a triangle with the edge $(v,u) \in E$, and let S_v and S_u be the set of nodes that form a 2-star with v and u, respectively. Furthermore, E_c is the set of edges that complete a 4-cycle with respect to the edge $e = (v,u)$ where for each edge $(r,s) \in E_c$ such that $r \in S_v$ and $s \in S_u$ and both $(r \cap S_u) \cup (s \cap S_v) = \emptyset$.

any arbitrary function/weight computed on the graph G. One possibility is to use uniform sampling probabilities such that each p_i is

$$p_i = |J|/|E|. \tag{15}$$

Intuitively, p_i is the fraction of edge neighborhoods selected thus far. Results for both uniform and nonuniform sampling probabilities are discussed and investigated in Section IV. In addition, let σ_i be defined as

$$\sigma_i = \frac{1}{p_i}$$

where σ_i is the inverse sampling probability of graphlet i used to correct the sampling bias. This corresponds to the Horvitz–Thompson construction [36], [50]. Let us note that in Algorithm 2, the cliques and cycles are computed via Algorithms 3 and 4 using information from the $(k-1)$-graphlets. However, when memory is limited, then Algorithms 5 and 6 should be used. These methods search over the sets T_e, S_u, and S_v from the $(k-1)$-graphlets directly using binary search.

Error Analysis: Let $Y_i(e)$ be the true count of an arbitrary-induced subgraph $G_i \in \mathcal{G}$ if and only if the subgraph is incident to e, then $Y_i = \sum_{e \in E} Y_i(e)$. Assume that we sample a set of edge neighborhoods with probability ϕ, then $X_i = \sum_{e \in J} (Y_i(e)/\phi)$ where X_i is an estimator for $\mathcal{G}_i$. $\mathbb{E}[X_i] = Y_i$ is an unbiased estimate. The proof is as follows:

$$\mathbb{E}[X_i] = \mathbb{E}\left[\sum_{e \in J} \frac{Y_i(e)}{\phi}\right] = \sum_{e \in J} \mathbb{E}\left[\frac{Y_i(e)}{\phi}\right] \tag{16}$$

$$= \sum_{e \in E} \frac{\mathbb{E}[\mathcal{I}_e]}{\phi} \cdot Y_i(e) = \sum_{e \in E} \frac{Y_i(e)}{\phi} \cdot \phi = Y_i \tag{17}$$

where $\mathcal{I}_e$ is a Bernoulli random variable that indicates whether e and its neighborhood is sampled. Furthermore, the mean squared error $\text{MSE}(X_i)$ is

$$\mathbb{E}[(X_i - Y_i)^2] = \underbrace{\mathbb{V}[X_i]}_{\text{Variance}} + \underbrace{(\mathbb{E}[X_i] - Y_i)^2}_{\text{Bias}} \tag{18}$$

where $\mathbb{V}[X_i]$ is the variance component and $(\mathbb{E}[X_i] - Y_i)^2$ is the bias component of the estimator X_i. Therefore, $\text{MSE}(X_i) = \mathbb{V}[X_i]$ since X_i is an *unbiased estimator*.

Complexity: Let $T_{\max}$ and $S_{\max}$ denote the maximum number of triangles and stars incident to a selected edge $e \in J$. Note that $S_{\max}$ in reality is much smaller since for each edge $e = (v,u) \in J$, Algorithm 2 computes only S_u[8] such that $d_u \leq d_v$, and thus, $|S_u| \leq |S_v|$. For a single $\Gamma(e)$, Algorithm. 2 counts 4-cliques and 4-cycles centered at e in $\mathcal{O}(\Delta T_{\max})$ and $\mathcal{O}(\Delta S_{\max})$, respectively. From either 4-cliques/cycles, we derive all other graphlet counts in $o(1)$ using combinatorial relationships along with the $(k-1)$-graphlets. Thus, Algorithm 2 counts all graphlets for $\{\Gamma(e_1), \ldots, \Gamma(e_K)\}$ up to $k = 4$ in

$$\mathcal{O}(K\,\Delta T_{\max} + K\,\Delta S_{\max}) = \mathcal{O}(K\,\Delta(T_{\max} + S_{\max})).$$

Using K processing units (cores and workers), this reduces to $\mathcal{O}(\Delta(T_{\max} + S_{\max}))$. Our approach is also space efficient and requires a lot less space than the existing approaches [25], [26], [47], [48]. In particular, the space complexity of Algorithm 2 is $\mathcal{O}(N + 2\Delta - 1) = \mathcal{O}(N)$ using a hash table Ψ of size $N = |V|$ (Algorithms 3 and 4) or $\mathcal{O}(3\Delta - 1) = \mathcal{O}(\Delta)$ using binary search over T or S_u and S_v directly (Algorithms 5 and 6).

[8] As opposed to both S_u and S_v.

Algorithm 3 Clique counts via neigh-iter

```
1: procedure CLIQUE(Ψ, T_e)
2:     Set K_e ← 0
3:     parallel for each w ∈ T_e do
4:         for each r ∈ Γ(w) where Ψ(r) = λ_3 do set K_e ← K_e + 1
5:         Reset Ψ(w) to 0
6:     return K_e
```

Algorithm 4 Cycle counts via neigh-iter

```
1: procedure CYCLE(Ψ, S_u)
2:     Set C_e ← 0
3:     parallel for each w ∈ S_u do
4:         for each r ∈ Γ(w) where Ψ(r) = λ_2 do set C_e ← C_e + 1
5:         Reset Ψ(w) to 0
6:     return C_e
```

Algorithm 5 Clique counts restricted to searching T_e

```
1: procedure CLIQUERES(Ψ, T_e )
2:     Set K_e ← 0
3:     parallel for each vertex w_i in an ordering w_1, w_2, ··· of T_e do
4:         for each w_j ∈ {w_{i+1}, ..., w_{|T_e|}} in order do
5:             if w_i ∈ Γ(w_j) via binary search then K_e ← K_e + 1
6:     return K_e
```

Algorithm 6 Cycle counts restricted to S_u and S_v

```
1: procedure CYCLERES(Ψ, S_u, S_v )
2:     Set C_e ← 0
3:     parallel for each w ∈ S_u do
4:         for all r ∈ S_v do
5:             if r ∈ Γ(w) via binary search then C_e ← C_e + 1  ▷ 4-cycle
6:     return C_e
```

E. Estimation of Local Graphlet Statistics

This section formulates the local graphlet estimation problem, then describes a computational framework for estimating local graphlet statistics. The experiments in Section IV-E demonstrate the effectiveness of these methods. Computing *local graphlet statistics* $\mathbf{x}_i$ for an individual edge $e_i \in E$ (or node) in G (as opposed to the global graph G) is important with numerous potential applications. For instance, they can be used as powerful discriminative features $\{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_M\}$ for improving statistical relational learning (SRL) tasks [52] such as relational classification [46], link prediction, and weighting tasks (e.g., recommending items, friends, web sites, music, events, etc.) [53] detecting anomalies in graphs (e.g., detecting fraud, or attacks/malicious behavior in computer networks) [21], [22], among many others [44], [45], [54]. However, it is often expensive and computationally prohibitive to compute such local graphlet statistics in large networks. In this paper, we propose a local graphlet estimation framework that derives accurate approximations of the local graphlet statistics while being orders of magnitude faster than exact methods.

Definition 3 (LOCAL GRAPHLET ESTIMATION): *Given a graph $G = (V, E)$ and an edge $e_i = (v, u) \in E$, the* local graphlet estimation problem *is to find*

$$\mathbf{x}_i = [x_1 \;\; x_2 \;\; x_3 \;\; \cdots \;\; x_6 \;\; x_7 \;\; \cdots]^T \tag{19}$$

where $\mathbf{x}_i$ is an approximation of the exact local graphlet statistics denoted by $\mathbf{y}_i$ for edge e_i such that $\mathbb{D}(\mathbf{x}_i \parallel \mathbf{y}_i)$ is minimized (i.e., $\mathbf{x}_i \approx \mathbf{y}_i$) as well as the computational cost associated with the estimation.

The aim of the *local graphlet estimation problem* is to compute a fast yet accurate approximation of the graphlet statistics (such as counts) centered at an individual edge. Note that $\mathbb{D}(\mathbf{x}_i \parallel \mathbf{y}_i)$ in Definition 3 can be any loss function. Instead of approximating all graphlets up to size k, one may relax the above-mentioned problem to estimate a single graphlet pattern $G_j \in \mathcal{G}$ of interest (e.g., 4-node cliques).

A general estimation framework for the *local graphlet estimation problem* is shown in Algorithm 7. In particular, Algorithm 7 takes as input an edge e_i, a graph G or $\mathbf{\Gamma}(e_i)$ (neighborhood subgraph of e_i), a sampling probability p_e, and it returns the graphlet feature vector $\mathbf{x}_i \in \mathbb{R}^\kappa$ for $e_i \in E$ where $\kappa = |\mathcal{G}|$. This generalization gives rise to a highly expressive unifying *local graphlet estimation framework* with many interchangeable components. For computing the local graphlet statistics in Algorithm 7, any edge-centric method can be used such as PGD [13], [14], VCP [8], [23], Orca [28], or any future state-of-the-art approach. In this paper, we use the PGD library [13] to compute the local graphlet statistics required for estimation. Moreover, the class of local graphlet approximation methods has many attractive properties such as unbiasedness and consistency.

We now discuss Algorithm 7 in detail. In particular, Algorithm 7 shows how to efficiently estimate all graphlets of size $k \in \{2, 3, 4\}$ for an edge $e_i \in E$. First, we compute T_e, S_u, and S_v in Lines 3–9. Then, we use these sets to derive all graphlets of size $k = 3$ exactly in a constant time

Algorithm 7 Family of localized graphlet estimation (LGE) methods for accurate and unbiased estimation of *local graphlet properties*. Given an edge e_i or edge-induced subgraph $\mathbf{\Gamma}(e_i)$ and a sampling probability p_e, the general approach returns the estimated graphlet feature vector $\mathbf{x} = \mathbf{x}_i$ for $e_i \in E$

1: **procedure** LOCALGRAPHLETESTIMATION($\mathbf{\Gamma}(e_i)$ or G, e_i, p_e)
2: Initialize variables
3: **parallel for each** $w \in \Gamma(v)$ **do**
4: **if** $w \neq u$ **then** $S_v \leftarrow S_v \cup \{w\}$ and $\Psi(w) = \lambda_1$
5: **parallel for each** $w \in \Gamma(u)$ **and** $w \neq v$ **do**
6: **if** $\Psi(w) = \lambda_1$ **then**
7: $T_e \leftarrow T_e \cup \{w\}$ and set $\Psi(w) = \lambda_3$ ▷ triangle
8: $S_v \leftarrow S_v \setminus \{w\}$
9: **else** $S_u \leftarrow S_u \cup \{w\}$ and set $\Psi(w) = \lambda_2$ ▷ wedge
10: $x_2 = |T_e|$ ▷ triangles/3-cliques
11: $x_3 = (d_u + d_v - 2) - 2|T_e|$ ▷ 2-stars
12: **parallel for each** $w \in T_e$ **do**
13: **for** $j = 1, \ldots, \lceil d_w \cdot p_e \rceil$ **do**
14: Select a vertex $r \in \Gamma(w)$ via an arbitrary distribution $\mathbb{F}$
15: **if** $\Psi(r) = \lambda_3$ **then** Set $x_4 \leftarrow x_4 + (d_w / \lceil d_w \cdot p_e \rceil)$ ▷ 4-clique
16: Set $\Psi(w)$ to λ_4
17: $x_5 = \binom{|T_e|}{2} - x_4$ ▷ chordal-cycles
18: **parallel for each** $w \in S_u$ **do**
19: **for** $j = 1, \ldots, \lceil d_w \cdot p_e \rceil$ **do**
20: Select a vertex $r \in \Gamma(w)$ via an arbitrary distribution $\mathbb{F}$
21: **if** $\Psi(r) = \lambda_1$ **then** set $x_7 \leftarrow x_7 + (d_w / \lceil d_w \cdot p_e \rceil)$ ▷ 4-cycle
22: **if** $\Psi(r) = \lambda_2$ **then** set $x_6 \leftarrow x_6 + (d_w / \lceil d_w \cdot p_e \rceil)$ ▷ tailed-tri
23: Set $\Psi(w)$ to 0
24: **parallel for each** $w \in S_v$ **do**
25: **for** $j = 1, \ldots, \lceil d_w \cdot p_e \rceil$ **do**
26: Select a vertex $r \in \Gamma(w)$ via an arbitrary distribution $\mathbb{F}$
27: **if** $\Psi(r) = \lambda_1$ **then** set $x_6 \leftarrow x_6 + (d_w / \lceil d_w \cdot p_e \rceil)$ ▷ tailed-tri
28: Set $\Psi(w)$ to 0
29: $x_8 = \binom{|S_v|}{2} + \binom{|S_v|}{2} - x_6$ ▷ 3-stars
30: $x_9 = (|S_v| \cdot |S_u|) - x_7$ ▷ 4-paths
31: **return** $\mathbf{x}$, where x_k is the estimate of graphlet G_k for e_i

(Lines 10 and 11) as done in [13] and [14]. Note that these sets are computed exactly and up to this point, corresponds exactly to the exact algorithm given in [13]. Next, we estimate 4-cliques in Lines 12–16. In particular, Line 12 searches each vertex $w \in T_e$ in parallel. Given $w \in T_e$, we sample a neighbor $r \in \Gamma(w)$ with probability p_e accordingly to an arbitrary weighted/uniform distribution $\mathbb{F}$. Then, we check if r is of type λ_3 (from Line 7), as this indicates that r also participates in a triangle with $e = (v, u)$, and since $r \in \Gamma(w)$, then $\{v, u, w, r\}$ is a 4-clique. Line 16 ensures that the same 4-clique is not counted twice. Chordal cycles are estimated in Line 17. Furthermore, 4-node cycles are estimated in Lines 18–23 as well as a fraction of the tailed triangles. The other tailed triangles are estimated in Lines 24–28. Finally, the remaining graphlets are estimated in $o(1)$ time (Lines 29 and 30) using knowledge from the previous steps. Note that if $p_e = 1$ and sampling is performed without replacement, then Algorithm 7 reverts back to the exact method proposed in [13] and [14].

We can also use Hoeffding's inequality [55] to obtain estimates with provable error bounds. For instance, if we replace $\lceil d_w \cdot p_e \rceil$ everywhere in Algorithm 7 with $\lceil 0.5\epsilon^{-2} \ln(2/\delta) \rceil$, then the error rate of the estimate is at most ϵ with confidence

TABLE III
COMPUTATIONAL COMPLEXITY

Graphlet	Global	Local
4-clique	$\mathcal{O}(K\Delta T_{\max})$	$\mathcal{O}(\Delta_{\text{ub}} \cdot \lvert T_e \rvert)$
4-cycle	$\mathcal{O}(K\Delta S_{\max})$	$\mathcal{O}(\Delta_{\text{ub}} \cdot \lvert S_u \rvert)$
tailed-tri	$\mathcal{O}(K\Delta S_{\max})$	$\mathcal{O}\big(\Delta_{\text{ub}} \cdot (\lvert S_u \rvert + \lvert S_v \rvert)\big)$
all	$\mathcal{O}\big(K\Delta(S_{\max} + T_{\max})\big)$	$\mathcal{O}\big(\Delta_{\text{ub}}(\lvert S_u \rvert + \lvert S_v \rvert + \lvert T_e \rvert)\big)$

at least $1 - \delta$ [56]. The error rate ϵ and confidence level δ are specified by the user and given as input into Algorithm 7 (instead of p_e).

Complexity: The computational complexity is summarized in Table III. Note that just as before, we only need to compute a few graphlets and can directly obtain the others in a constant time. To compute all local graphlet statistics for a given edge, it takes: $\mathcal{O}(\Delta_{\text{ub}}(|S_u|+|S_v|+|T_e|))$ where Δ_{ub} is the maximum degree from any vertex in S_v, S_u, and T_e. Alternatively, we can place an upper bound Δ_{ub} on the number of neighbors searched from any vertex in S_v, S_u, and T_e. This can drastically reduce the time. The intuition is that for vertices with large neighborhoods, we only need to observe a relatively small (but representative) fraction of it to accurately extrapolate to the unobserved neighbors and their structure.

F. Discussion

The proposed family of LGE methods easily generalizes to graphlets of arbitrary size by replacing the definition of an edge-centric neighborhood with the more general and suitable notion of an edge ℓ-neighborhood

$$\Gamma_\ell(v, u) = \{w \in V \setminus \{v, u\} \,|\, D(v, w) \leq \ell \vee D(u, w) \leq \ell\}$$

where $\Gamma_\ell(v, u)$ represents the set of vertices with distance less than or equal to ℓ from $e = (v, u) \in E$. Thus, we set $\ell = 1$ for graphlets of size $k \leq 4$, and $\ell = 2$ for graphlets of size $k = 5$, and so on. Investigating the methods for graphlets of size 5 and above is left for the future work. The LGE framework also naturally allows for both uniform and weighted sampling designs, and has many other interchangeable components as well. Note that if the total number of edges is unknown (due to streaming, problem constraints, or other issues), then Algorithm 1 is easily adapted, e.g., one may simply specify the number of graphlets to sample (instead of the fraction of graphlets to sample denoted by ϕ in Algorithm 1). Unlike the existing work, the proposed LGE methods are naturally amenable to streaming graphs and for graphs too large to fit into memory. For instance, we do not need to read the entire graph into memory, as long as there is an efficient way to obtain the ℓ-neighborhood subgraph $\mathbf{\Gamma}(e_i)$ required for estimation.

In this paper, we leveraged PGD [13] to count the graphlets in the sampled neighborhood subgraph. However, the proposed estimation framework is flexible for use with other exact subgraph counting algorithms including Orca [28], VCP [8], [23], or any future state-of-the-art approach. Therefore, the fastest state-of-the-art enumeration approach can always be used by the framework (see Step 3 in Fig. 1) to speedup the estimation even further. In other words, the framework is independent of the exact enumeration approach used.

In the interest of space and to keep the presentation simple, we have left out several details on performance enhancement that we have in our implementation. To give a small example, we use an adjacency matrix structure for small graphs in order to facilitate $o(1)$ edge checks. For larger graphs, we efficiently encode the neighbors of the top-k vertices with the largest degree (and relabel to save space/time) for $o(1)$ graph operations. We use a fast $O(d)$ neighborhood set intersection procedure to dynamically select local search procedures over T_e, S_u, and have many other optimization's throughout the code (bit-vector graph representation, etc.).

III. PARALLELIZATION

Estimation methods from the framework are parallelized via independent edge-centric graphlet computations over the selected set of edge-induced neighborhoods $\{\Gamma(e_i), \ldots, \Gamma(e_K)\}$. The parallelization is described such that it could be used for both shared and distributed memory architectures.[9] The parallel constructs used are a worker task queue and a global broadcast channel. Multithreaded Message Passing Interface is used for an intermachine communication. We assume each machine q has a queue and a copy of the graph[10] shared among the set of local workers (processing units). For global graphlet statistics, the communication cost for a single worker is $O(|\mathcal{G}|)$.

The main parallel loop can be viewed as a task generator that farms the next b edges out to a worker, which then computes the graphlets centered at each of the b edge neighborhoods. Edge neighborhoods are dynamically partitioned to workers by "hardness" where the most difficult edge neighborhood is assigned to the first worker, the second most difficult is assigned to the second worker, and so on. This ensures that we avoid common problems present in other approaches such as the curse of the last reducer [57] (due to the power-law observation [58]).

The existing state-of-the-art estimation methods are based on sequential algorithms which are inherently slow, difficult to parallelize, and have t dependent parts due to implementation issues, among others. Furthermore, our edge-centric parallel estimation method provides a better load balancing (compared to vertex-based approaches). It is straightforward to see that if $N < M$, then our approach requires less computations per edge than per vertex since

$$X_i = \sum_{e \in E}^{M} X_i(e) = \sum_{v \in V}^{N} X_i(v). \tag{20}$$

Parallelizing via edge-induced neighborhoods provides much better load balancing for real-world sparse graphs that follow

[9]In the context of message passing and distributed memory parallel computing, a nodeers to another machine on the network (or bus) with its own set of memory, and multicore CPUs, etc.

[10]For implementation on parallel computing architectures with limited memory, one only needs to transfer the set of edge-induced neighborhood subgraphs, which can be streamed if needed.

a power law. The time taken to count graphlets for each edge obeys a power law with only a few edges taking much longer than the others (as observed in [58]). In addition, each $\Gamma(e)$ graphlet computation may be easily split into t independent tasks, e.g., 4-cliques (Algorithm 3), 4-cycles (Algorithm 4), solving the linear system, etc. Moreover, the edge-centric estimation methods are useful for situations where one might only be able to retrieve the (induced) neighborhood of an edge due to privacy or data collection issues, etc. In addition, our approach does not require storage, knowledge, and preprocessing of the entire graph (as opposed to the existing work). Other important properties include the neighborhood search order Π, the batch size b, and the dynamic assignment of jobs (for load balancing). As an aside, there have been a few distributed memory [59] and shared memory [60], [61] exact algorithms. However, these algorithms are based on older inefficient *exact enumeration* algorithms, whereas this paper is focused on the *estimation* methods. In addition, these approaches are all vertex-centric, as opposed to our edge-centric approach, and mainly focus on finding network motifs, i.e., statistically significant subgraph patterns.

IV. Experiments

In this section, we evaluate the empirical error and performance of the methods with extensive experiments on over 300 networks (real world and synthetic) from more than 20 domains with different structural characteristics. All data are available at Network Repository [62]. Unless otherwise mentioned, we use PGD [13] to compute the exact graphlet counts for comparison.

A. Estimating Global Graphlet Statistics

We proceed by first demonstrating the effectiveness of the proposed methods for estimating the frequency of graphlets up to size $k = 4$. Given an estimated statistic X_i of an arbitrary graphlet $G_i \in \mathcal{G}$, we consider the relative error

$$\mathbb{D}(\, X_i \parallel Y_i \,) = \frac{|X_i - Y_i|}{Y_i} \tag{21}$$

where Y_i is the actual statistic (e.g., frequency) of G_i. Thus, this is a measure of how far the estimated statistic is from the actual graphlet statistic. Note X_i is the mean estimated value across 100 independent runs. The relative error indicates the quality of an estimated graphlet statistic relative to the magnitude of the exact statistic. Results for the most difficult graphlet (4-clique) are provided in Table IV for a wide range of graphs from various domains. Note that the approach provides even better estimates for the other graphlets. Overall, the results demonstrate the effectiveness of the estimation methods as they have excellent empirical accuracy. Furthermore, the estimation error for the disconnected graphlets is considerably smaller than the error for connected graphlets.

We also estimated univariate graphlet statistics beyond simple global counts such as the median, standard deviation, variance, interquartile range, Q1, Q3, and others. Overall, the methods are found to be accurate for many of the new graphlet statistics as shown in Fig. 4. For estimating the maximum # of 4-node cliques that any edge participates, we also observed that selecting edges via the k-core distribution resulted in high accuracy at very low sample rates.

TABLE IV

Estimates of Expected Value and Relative Error

Estimates of expected value and relative error using 100K samples. The graphlet statistic for the full graph is shown in the first column. β_{lb} and β_{ub} are 95% lower and upper bounds, respectively. Note M=million (mega), B=billion (giga).

	graph	Y	X	$\frac{\lvert Y-X\rvert}{Y}$	β_{lb}	β_{ub}
4-CLIQUE	ca–citeseer	18.7M	18.7M	0.0004	18.3M	19M
	ca–dblp-2012	16.7M	16.7M	0.0004	16M	17.3M
	soc–flickr	1.7B	1.7B	0.0003	1.7B	1.7B
	soc–friendster	9B	9B	0.0038	8.9B	9.1B
	soc–gowalla	6M	6M	0.0009	5.9M	6.2M
	soc–orkut	3.2B	3.2B	0.0016	3.1B	3.3B
	soc–pokec	42.9M	42.9M	0.0002	41.9M	43.9M
	socfb–Berkeley13	26.6M	26.6M	0.0007	26.2M	27M
	socfb–Indiana	60.1M	60.1M	0.0004	59.3M	61M
	socfb–MIT	13.6M	13.6M	0.0004	13.5M	13.8M
	socfb–OR	13.3M	13.3M	0.0005	13.1M	13.5M
	socfb–Texas84	70.7M	70.7M	0.0002	69.6M	71.8M
	socfb–UCLA	28.6M	28.6M	0.0005	28.2M	29M
	socfb–UCSB37	18.1M	18.1M	$<10^{-4}$	17.9M	18.4M
	socfb–UF	97.9M	97.9M	0.0001	96.5M	99.3M
	socfb–UIllinois	64M	63.9M	0.0008	63M	64.9M
	socfb–Wisconsin87	23M	23M	0.0011	22.7M	23.3M
	web–wikipedia2009	1.4M	1.4M	0.0004	1.3M	1.5M

B. Confidence Bounds

Given an arbitrary graphlet $G_i \in \mathcal{G}$, we compute X_i using the estimators from the framework derived in Section II and construct confidence bounds for the unknown Y_i. Using the large sampling distribution, we derive lower and upper bounds such that

$$\beta_{\text{lb}} \leq Y_i \leq \beta_{\text{ub}} \tag{22}$$

where

$$\beta_{\text{lb}} = X_i - z_{\alpha/2} \cdot \sqrt{\mathbb{V}[X_i]} \tag{23}$$

and

$$\beta_{\text{ub}} = X_i + z_{\alpha/2} \cdot \sqrt{\mathbb{V}[X_i]}. \tag{24}$$

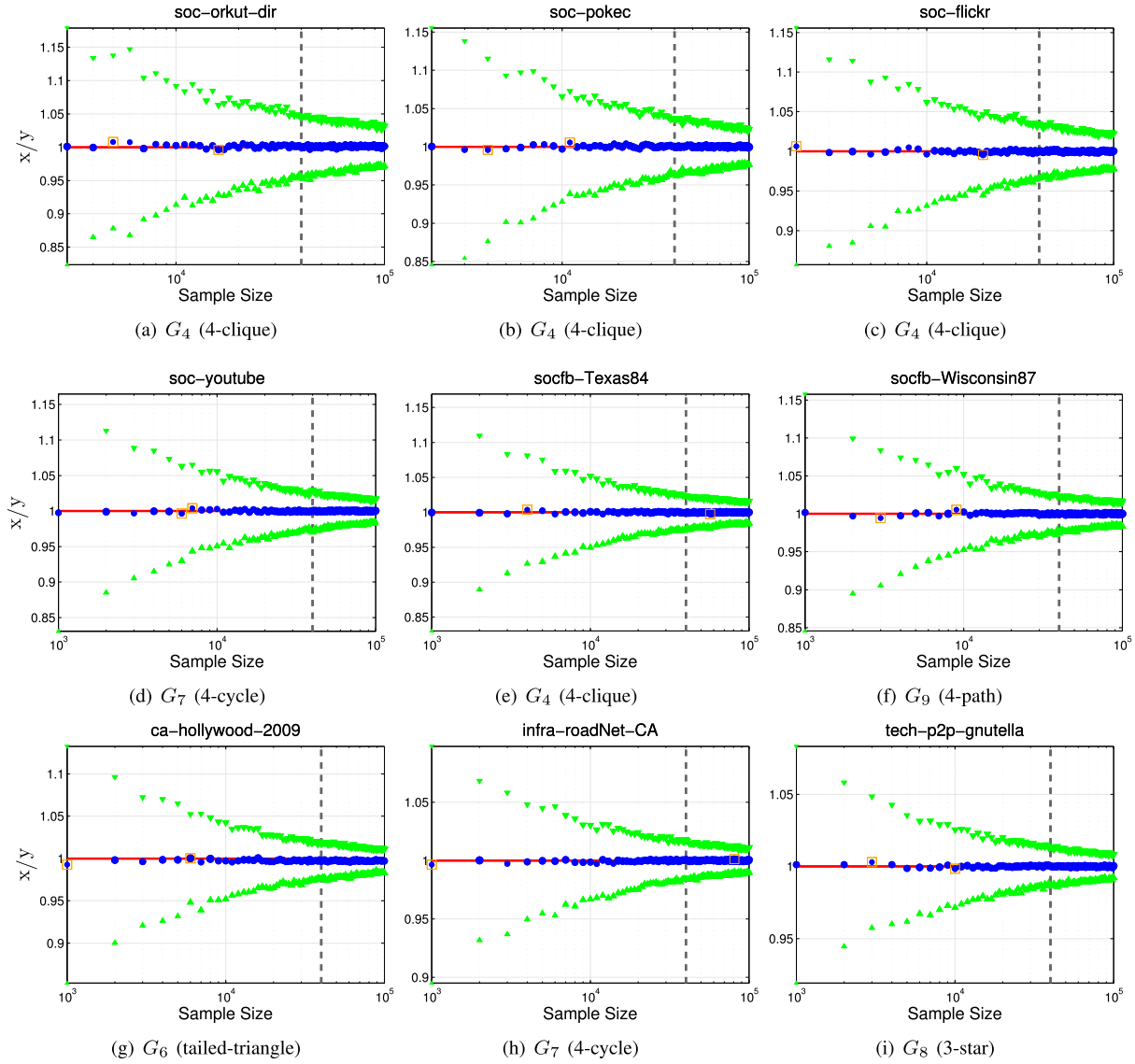
The estimates X_i and $\mathbb{V}(X_i)$ are computed using the equations of the unbiased estimators of counts and their variance. Thus, $\alpha = 0.05$ and $z_{\alpha/2} = z_{0.025} = 1.96$ for a 95% confidence interval for the unknown Y_i. This gives

$$X_i - 1.96\sqrt{\mathbb{V}[X_i]} \leq Y_i \leq X_i + 1.96\sqrt{\mathbb{V}[X_i]}. \tag{25}$$

Furthermore, the sample size needed is $K = (z_{\alpha/2} \cdot (\mathbb{V}[X_i])^{1/2}/\alpha/2)^2$.

The 95% upper and lower bounds (i.e., β_{ub} and β_{lb}) for the 4-clique are given in Table IV (other graphlet results were removed due to space). In all cases, the actual graphlet statistics lie inside the error bounds, $\beta_{\text{lb}} \leq Y_i \leq \beta_{\text{ub}}$. Fig. 3 investigates the properties of the sampling distribution as the sample size increases. The circle (blue) in Fig. 3 represents the fraction X_i/Y_i. Furthermore, β_{lb}/Y_i and β_{ub}/Y_i are represented in Fig. 3 by $\triangle$ and $\triangledown$, respectively. The key findings are summarized as follows:

- The sampling distribution is centered and balanced over the actual graph statistic (represented by the red line).
- Upper and lower bounds always contain the actual value.
- As the sample size increases, the bounds *converge* to the actual value of the graphlet statistic. The *estimated* variance decreases as k grows larger.



(a) G_4 (4-clique) (b) G_4 (4-clique) (c) G_4 (4-clique)

(d) G_7 (4-cycle) (e) G_4 (4-clique) (f) G_9 (4-path)

(g) G_6 (tailed-triangle) (h) G_7 (4-cycle) (i) G_8 (3-star)

Fig. 3. Confidence bounds for a variety of graphlets. We used graphs from a variety of domains and types. Note that 4-cliques is often the most difficult to estimate, and thus, we have dedicated more results for these hard instances. The properties of the sampling distribution and convergence of the estimates are investigated as the sample size increases. Circle (•): X/Y (y-axis). ▲ and ▼: β_{lb}/Y and β_{ub}/Y, respectively. Square (□): min/max X/Y. Gray dashed vertical line: sample at 40K edges. Note that the method has excellent accuracy even at this small sample size.

- Confidence bounds are within 5% of the actual for all graphs and subgraph patterns.
- Thus, the sampling distribution of the estimation framework has many attractive properties including unbiased estimates for all subgraph patterns and low variance even for very small sample sizes (and variance decreases as a function of the sample size).

Let $\mathbb{P}(\beta_{\text{lb}} \leq Y \leq \beta_{\text{ub}})$ be the exact coverage probability of our bounds. We observe that the confidence bounds are tight (for all subgraph patterns) and holds to a good approximation that is within $\pm 5\%$ of the actual value for all 300+ graphs.

C. Estimating Graphlet Frequency Distributions

We investigate the methods for estimating the GFDs from a wide variety of networks with different structural characteristics including real-world and synthetic graphs. Exact graphlet counts are computed using PGD [13] for comparison. Strikingly, the estimated GFD from our approach almost perfectly matches the actual GFD (Fig. 5). Observe that the methods are evaluated by how well they estimate the entire exact GFD, and thus, Fig. 5 indicates that the proposed methods estimate all such induced subgraphs from Table I with an excellent accuracy (matching the actual GFD in all cases). Results for a variety of sparse real-world graphs from different domains are given in Table V. Overall, most graphlet estimates in Table V have relative error less than 10^{-4}. In all cases, we find no significant difference between the estimate and the actual (Table V). In Table VI, we also report results on a standard collection synthetic benchmark graphs from the DIMACS

	mean	median	std	var	iqr	q1	q3
0.1	0.0002	0.0009	0.0009	0.002	0.010	0.015	0.0046
0.01	0.0026	0.0167	0.0125	0.025	0.003	0.020	0.0051

Fig. 4. Estimation error for a variety of univariate statistics for the local 4-clique graphlet distribution. These results are from socfb–MIT, and thus, even a sample size of 1% is small.

TABLE V

GFD ESTIMATES FOR A WIDE VARIETY OF SPARSE REAL-WORLD NETWORKS

All graphlet estimates have less than 10^{-3} relative error and those with relative error $<10^{-4}$ are highlighted. The KS test was used to test for significance of differences between the estimated and true distributions, and the test results show that they are significantly similar with 99% confidence (p-value < 0.01). Exact graphlet counts are computed using PGD [13] for comparison.

Graph	$\|E\|$							KS-Stat.
ca-AstroPh	196.9K	0.010	0.016	0.193	0.001	0.324	0.455	$<10^{-4}$
ca-MathSciNet	820.6K	0.001	0.003	0.077	<0.001	0.461	0.457	$<10^{-4}$
ia-email-EU	54.3K	<0.001	0.001	0.031	<0.001	0.715	0.252	0.0005
ia-enron-large	180.8K	<0.001	0.004	0.060	0.001	0.716	0.219	$<10^{-4}$
rt-retweet-crawl	2.2M	<0.001	<0.001	<0.001	<0.001	0.898	0.101	$<10^{-4}$
soc-douban	327.1K	<0.001	<0.001	0.012	<0.001	0.436	0.552	0.0005
soc-youtube-s	2.9M	<0.001	<0.001	0.002	<0.001	0.982	0.016	0.0003
soc-flickr	3.1M	0.003	0.020	0.132	0.010	0.477	0.358	0.0007
soc-twitter-higgs	14.8M	<0.001	<0.001	0.003	<0.001	0.972	0.024	$<10^{-4}$
soc-friendster	1.8T	<0.001	<0.001	0.009	<0.001	0.400	0.590	$<10^{-4}$
socfb-UIllinois	1.2M	0.001	0.005	0.071	0.002	0.499	0.422	0.0001
socfb-Indiana	1.3M	0.001	0.006	0.089	0.003	0.300	0.600	$<10^{-4}$
socfb-Penn94	1.3M	<0.001	0.002	0.039	0.001	0.652	0.304	$<10^{-4}$
socfb-Texas84	1.5M	<0.001	0.002	0.043	0.001	0.667	0.287	0.0007
tech-internet-as	85.1K	<0.001	<0.001	0.005	<0.001	0.963	<0.001	0.0003

TABLE VI

GFD ESTIMATES FOR DENSE SYNTHETIC GRAPHS FROM DIMACS

GFD estimates for dense synthetic graphs from the DIMACS NP-Hard Problem Challenge described in [64], [65]. All graphlet estimates have less than 10^{-3} relative error and those with relative error $<10^{-4}$ are highlighted. The KS test was used to test for significance of differences between the estimated and true distributions, and the test results show that they are significantly similar with 99% confidence (p-value < 0.01).

Graph	$\|E\|$							KS-Stat.
C2000-5	999.8K	0.026	0.158	0.316	0.079	0.105	0.316	$<10^{-4}$
C4000-5	4M	0.026	0.158	0.316	0.079	0.105	0.316	$<10^{-4}$
p-hat1500-1	284.9K	0.004	0.047	0.218	0.048	0.190	0.494	0.0010
johnso32-2-4	107.8K	0.446	0.428	0.066	0.033	0.023	0.005	$<10^{-4}$
brock800-3	207.3K	0.089	0.290	0.314	0.079	0.057	0.170	$<10^{-4}$
brock800-1	207.5K	0.090	0.291	0.314	0.079	0.057	0.170	$<10^{-4}$
san1000	250.5K	0.120	0.192	0.274	0.037	0.063	0.315	$<10^{-4}$
sanr400-0-5	39.9K	0.027	0.159	0.316	0.079	0.105	0.314	0.0005
DSJC500-5	62.6K	0.027	0.159	0.316	0.079	0.105	0.314	$<10^{-4}$
hamming6-4	704	0.001	0.025	0.140	0.106	0.240	0.487	$<10^{-4}$

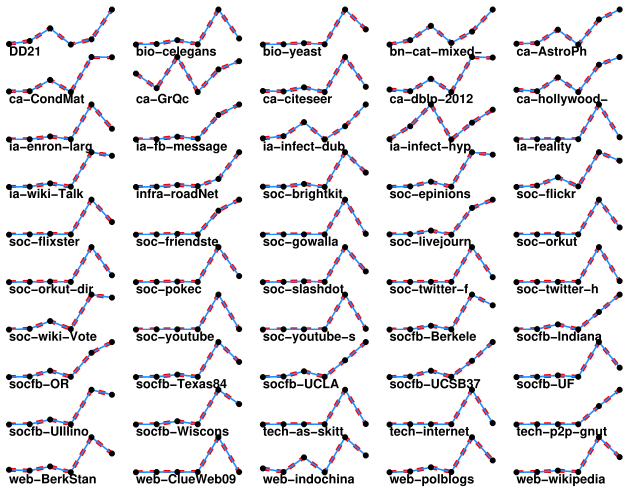


Fig. 5. Estimated GFD is indistinguishable from the actual (larger dotted red line), even across a wide variety of graphs with fundamentally different structural characteristics. The y-axis is the normalized 4-vertex graphlet counts $\mathbf{x}' = \mathbf{x} - \min(\mathbf{x}) / \max(\mathbf{x}) - \min(\mathbf{x})$ where $\mathbf{x}$ is the vector of graphlet counts. Nevertheless, similar results were found for other graphlet sizes and GFD variants.

NP-Hard Problem Challenge [63]. These graphs are *dense* and are used extensively for evaluating NP-hard problems such as finding the largest clique as described in [64] and [65]. Nevertheless, the estimators that are given in Table VI are to be highly accurate across all graphlets and graphs. Notably, the Kolmogorov–Smirnov-Statistic is very small for all graphs in both Tables V and VI.

In addition, we also studied the effectiveness of the estimation methods on synthetic graphs from a variety of well-known graph models including Erdős–Rényi (ER) [67] graphs, the geomertic random graphs (GEO) [65], scale-free Barabási–Albert (BA) [68] preferential attachment model, and the Kronecker graph model [66]. Results are reported in Table VII. The geometric random graph model networks GEO-15 to GEO-20 in Table VII are from the popular DIMACS 10 challenge [69], [70], whereas the Kronecker graphs 16–18 are from the Graph 500 supercomputer benchmark [71] (see [69]–[71] for more details). We also included a few other geometric random graphs (GEO 1–3) in Table VII; these graphs all have the same number of nodes but a different number of edges going from 100K to 200K in 50K increments. Overall, the estimation methods have an excellent accuracy (with very small relative error) across all synthetic graphs from the various graph models as observed in Table VII. Similar results were observed using other graph models such as Chung-Lu and Block Erdos-Renyi, and therefore, were removed for brevity. Many graphs and results were also removed due to space.

D. Scalability Results

This section investigates the scalability of the *parallel graphlet estimation methods*. We use speedup to evaluate the effectiveness of the parallel algorithm. Speedup is simply $S_p = (T_1/T_p)$, where T_1 is the execution time of the sequential algorithm and T_p is the execution time of the parallel algorithm with p processing units. For the results in Fig. 6, we used a

TABLE VII

GFD ESTIMATES OF SYNTHETIC GRAPHS FROM A VARIETY OF WELL-KNOWN SYNTHETIC GRAPH MODELS

GFD estimates of synthetic graphs from a variety of well-known *synthetic graph models* including the geomertic random graph model (GEO) [66], Kronecker graph model [67], Erdős-Rényi (ER) [68], and the Barabási-Albert (BA) [69] scale-free preferential attachment model. All graphlet estimates have less than 10^{-3} relative error and those with relative error $<10^{-4}$ are highlighted. The KS test was used to test for significance of differences between the estimated and true distributions, and the test results show that they are significantly similar with 99% confidence (p-value < 0.01). Exact graphlet counts are computed using PGD [13] for comparison.

Graph	$\|V\|$	$\|E\|$							KS-Stat.
GEO-1	1K	100K	0.051	0.114	0.343	0.006	0.080	0.407	$<10^{-4}$
GEO-2	1K	150K	0.067	0.137	0.365	0.007	0.074	0.349	$<10^{-4}$
GEO-3	1K	200K	0.092	0.166	0.383	0.008	0.065	0.286	$<10^{-4}$
GEO-15	32.7K	160.2K	0.057	0.111	0.326	0.003	0.048	0.455	0.0004
GEO-16	65.5K	342.1K	0.056	0.110	0.325	0.003	0.048	0.457	0.0008
GEO-20	1M	6.8M	0.056	0.111	0.325	0.003	0.048	0.456	$<10^{-4}$
Kron-16	55.3K	2.4M	<0.001	0.009	0.091	0.002	0.737	0.161	$<10^{-4}$
Kron-17	107.9K	5.1M	<0.001	0.006	0.076	0.002	0.765	0.151	0.0007
Kron-18	210.1K	10.5M	<0.001	0.005	0.063	0.001	0.790	0.141	$<10^{-4}$
ER-1	1K	100K	<0.001	0.019	0.149	0.037	0.199	0.596	$<10^{-4}$
ER-2	1K	150K	0.003	0.047	0.218	0.055	0.169	0.508	$<10^{-4}$
ER-3	1K	37.3K	<0.001	0.002	0.055	0.015	0.233	0.694	$<10^{-4}$
ER-4	10K	2.5M	<0.001	<0.001	0.038	0.009	0.238	0.714	$<10^{-4}$
ER-5	1M	5M	<0.001	<0.001	<0.001	<0.001	0.250	0.750	$<10^{-4}$
BA-1	1K	50.1K	0.002	0.021	0.153	0.021	0.278	0.525	$<10^{-4}$
BA-2	1K	100K	0.006	0.052	0.225	0.033	0.232	0.452	$<10^{-4}$
BA-3	1K	150K	0.015	0.092	0.275	0.042	0.199	0.377	$<10^{-4}$
BA-20-1	10K	199.6K	<0.001	<0.001	0.023	0.002	0.481	0.494	$<10^{-4}$
BA-40-1	10K	398.4K	<0.001	0.001	0.037	0.003	0.442	0.516	$<10^{-4}$
BA-80-1	10K	793.6K	<0.001	0.003	0.056	0.005	0.394	0.542	0.0006
BA-20-2	100K	1.9M	<0.001	<0.001	0.005	<0.001	0.657	0.338	$<10^{-4}$
BA-40-2	100K	3.9M	<0.001	<0.001	0.009	<0.001	0.601	0.390	$<10^{-4}$
BA-80-2	100K	5.1M	<0.001	<0.001	0.015	<0.001	0.607	0.378	0.0005

TABLE VIII

LOCAL GRAPHLET ESTIMATION RESULTS

For each graph problem, we report the relative error averaged over 500 randomly selected edges. These experiments use $p_e = 0.001$ (See Section II-E for more details). In addition to the high accuracy, the local graphlet estimation methods are between 900-1000 times faster, and thus fast and highly scalable.

	RELATIVE ERROR							
graph							**KL**	**L1**
soc-flickr	0.001	0.001	0.001	0.001	0.001	0.001	0.0001	$<10^{-4}$
bio-human-gene1	0.002	0.002	0.001	0.001	0.001	0.001	0.0004	$<10^{-4}$
tech-internet-as	0.0001	0.0001	0.0012	0.0002	0.001	0.0002	0.001	$<10^{-4}$
sc-nasasrb	0.004	0.004	0.001	0.002	0.003	0.002	0.004	0.001

4-processor Intel Xeon E5-4627 v2 3.3 GHz CPU. Overall, the methods show strong scaling (see Fig. 6). Similar results were found for other graphs and sample sizes.

E. Local Graphlet Estimation Experiments

This section investigates the accuracy, runtime, and scalability of the computational framework presented in Section II-E for estimating local graphlet statistics and distributions of individual graph elements such as an edge (or node, path, or subgraph) as opposed to estimating global graphlet statistics over the entire graph G. Results are given in Table VIII. Note that for simplicity, nodes are selected uniformly at random; thus, $\mathbb{F}$ in Algorithm 7 represents a uniform distribution over the neighbors.

F. Extremal Graphlet Estimation

Given a graph G, and a graphlet G_j of size k, the extremal (max) graphlet estimation problem is to find

$$Z_j = \max_{e_i \in \{e_1,\ldots,e_m\}} [X_j(e_i)] \tag{26}$$

where Z_j is the maximum number of times graphlet G_j occurs at any edge $e_i \in E$ in G. The aim is to compute the maximum frequency that graphlet G_j occurs at any edge $e_i \in E$ in G. For this problem, we leverage the proposed LGE framework from Section II and bias the estimation method toward selecting a small set of edge J where G_j is most likely to appear at larger frequencies. The set of edges J are sampled via a graph parameter/distribution that appropriately biases selection of edges that are most likely to induce large quantities of the graphlet G_j. For relatively dense graphlets such as the k-clique (or chordal-cycle/diamond, etc.), we investigated sampling edges from the largest k-core subgraphs. More specifically, instead of selecting edge neighborhoods via a uniform distribution $\mathbb{F}$, our approach replaces $\mathbb{F}$ in Line 2 of Algorithm 1 with a weighted distribution that biases the selection of edge neighborhoods toward those in large k-core subgraphs (i.e., edge neighborhoods centered at edges with large k-core numbers). Similarly, one may also use the triangle core subgraphs if computed to obtain an estimate with lower error. Results demonstrate the effectiveness of this approach in Table IX. Strikingly, the earlier approach finds the optimal solution (while taking only a fraction of the time) for many graphs as well as many of the k-vertex graphlets.

G. Comparison to Previous Work

To compare with the previous estimation methods, we measure the time required by each method to obtain an estimate with relative error less than 0.01 (accuracy greater than 0.99). This ensures the estimation methods are compared fairly. Notice that it does not make sense to compare the

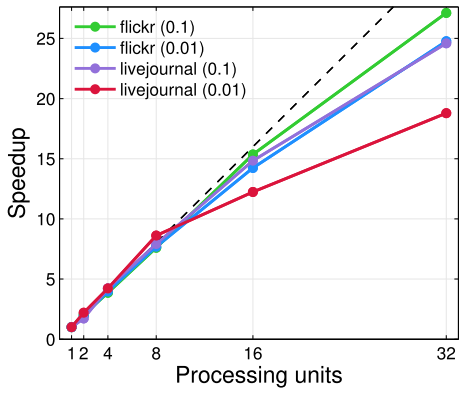


Fig. 6. Strong scaling results are observed across various sample sizes (see text for discussion).

TABLE IX
RESULTS FOR EXTREMAL GRAPHLET ESTIMATION

Results for two of the proposed techniques for estimating the maximum frequency of an arbitrary induced subgraph centered at an edge in G. The results below use $p_i = 0.005$ and are for socfb–Texas. Similar results were found with different graphs and sampling probabilities, and thus, removed for brevity. Note that the runtime is the total time taken to estimate all graphlet statistics. Clearly, selecting edge neighborhoods using the weighted probability distribution based on k-core numbers gives much better estimates for the vast majority of statistics below. In particular, uniform does better only for estimating the maximum 3-stars centered at any edge in G. Nevertheless, both are orders of magnitude faster than the exact method. For instance, the k-core approach is 157x faster than the exact method (on average), whereas the uniform method is 185x faster. Note that the best result among the estimation methods is bold, whereas * indicates that the estimate returned by the method is optimal (that is, it matches the actual maximum returned by the exact PGD [13] algorithm).

		Maximum graphlet counts					
Method	**Speedup**						
KCORE	157x	**45650***	**3.85M***	**26509***	**50351***	19.51M	**11.01M***
UNIFORM	185x	8172	22180	12112	24429	**19.89M**	3.35M
Exact	–	45650	3.85M	26509	50351	19.91M	11.01M

accuracy of an estimation method without taking into account runtime, since the accuracy (relative error) of an estimation method increases (decreases) as a function of time (or work performed). Obviously, if time is not considered, then one could simply use an exact method to achieve perfect accuracy. We also note that fixing the number of samples used by each method and measuring accuracy often leads to incorrect and misleading results since the accuracy depends on what each method calls a sample, and thus, a method may use significantly more work than another.

In Table X, we report the time each method takes to obtain an estimate with relative error less than 0.01 (accuracy greater than 0.99). As an aside, it is worth mentioning that the existing work is fundamentally different than ours, both in techniques, as well as in the estimation problems themselves. For instance, these methods estimate only simple global counts of graphlets, whereas the proposed class of LGE methods accurately estimates a wide variety of global and local statistics (including simple counts) and distributions (see Table II for a summary of the differences). Note that the 3-path sampling heuristic by Jha *et al.* [49] requires a lot more samples to obtain estimates with similar accuracy. In addition, that approach

TABLE X
RESULTS COMPARING LGE TO OTHER METHODS

Results for counting graphlets for four *massive networks* and one smaller graph (see text for discussion). For each method, we report the time required until the relative error is less than 0.01 (*i.e.*, accuracy is greater than 0.99). A hyphen (–) indicates that the method did not terminate within 12 hours (with relative error less than 0.01). The best time for each problem instance is in bold.

		Time in seconds				
graph	$\|E\|$	LGE	3-PATH	GUISE	GRAFT	PGD (exact)
soc–sinaweibo	261M	**12.3**	–	–	–	33359
web–ClueWeb09	7.81B	**65.6**	–	–	–	–
soc–friendster	1.81B	**44.1**	–	–	–	–
soc–twitter	1.20B	**341.2**	–	–	–	–
wiki–Talk	4.6M	**0.0007**	1.04	–	–	0.14

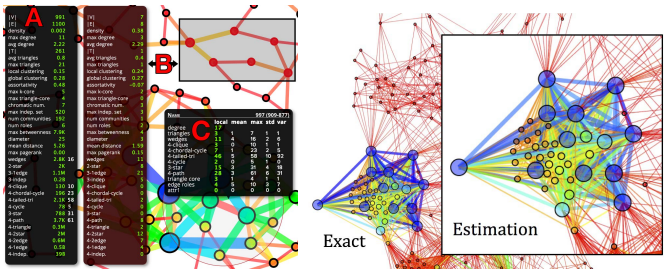


Fig. 7. Application of the estimation methods for real-time interactive graph mining and learning. Edges and nodes from a power-grid network [62] are colored/weighted by the estimated local 4-path count (left). (a) Estimated global graphlet counts and other statistics. (b) Summary statistics of the selected subgraph (rectangular region). (c) Local graphlet statistics (including frequency, mean, max, standard deviation, …) of the selected edge. Edges/nodes from tech-routers [62] are colored/weighted by the local 4-clique count (right). We observe that the visualizations using the exact and estimated graphlet features are strikingly similar, with trivial differences.

requires two different methods for estimating graphlet counts of size 4, and thus, requires 2× the samples. In particular, we find that 3-path sampling, GUISE [47], and GRAFT [48] are unable to obtain accurate estimates within a reasonable amount of time. Furthermore, GUISE and GRAFT did not converge, even despite using millions of samples, which is consistent with recent findings [49], and especially true for the massive networks used in this paper (see Table X). In some cases, the runtime of these methods even exceeded an exact graphlet algorithm, and thus these methods are not very useful in practice. Notably, our method is not only more accurate at lower sampling rates, but significantly faster than these methods. For instance, on soc–flickr we are 8047× faster than the path sampling heuristic. In some cases, we even find that our exact method is significantly faster than the 3-path heuristic (for instance, on wiki–talk and others). We also investigated selecting node-centric neighborhoods and other methods based on sampling graphlets directly, though the accuracy was worse in all cases, and thus removed for brevity.

H. Applications

This section uses the novel statistics and estimators for real-time interactive graph visualization and exploratory analysis. Graphlet estimators are implemented in a web-based *interactive* visual graph mining platform [72] called

GraphVis (Fig. 7). Across all experiments, the graphlet methods are fast and scalable taking <1 ms for 99% of the interactive queries and graphs, while also accurate (with no observable difference). Thus, the graphlet estimation methods are able to support *real-time* interactive queries for visual graph mining, exploration, and predictive modeling tasks (such as relational classification).

V. Conclusion

This paper proposed a general unbiased estimation framework called LGE for estimation of global and local graphlet properties (such as counts) in massive networks with billions of edges. The methods are shown to be accurate, fast, and scalable for both sparse and dense real-world and synthetic graphs of arbitrary size. Moreover, LGE has many interchangeable components and is effective for a wide variety of networks, applications, and domains, which have fundamentally different structural properties. We have shown that even for large networks with over a billion edges, one can compute graphlets fast and with low error. The newly introduced family of graphlet estimators greatly improves the scalability, flexibility, and utility of graphlets. Finally, the methods give rise to new opportunities and applications for graphlets (as shown in Section IV-H).

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