Moss: A Scalable Tool for Efficiently Sampling and Counting 4- and 5-Node Graphlets

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ABSTRACT
Counting the frequencies of 3-, 4-, and 5-node undirected motifs (also known as graphlets) is widely used for understanding complex networks such as social and biology networks. However, it is a great challenge to compute these metrics for a large graph due to the intensive computation. Despite recent efforts to count triangles (i.e., 3-node undirected motif counting), little attention has been given to developing scalable tools that can be used to characterize 4- and 5-node motifs. In this paper, we develop computational efficient methods to sample and count 4- and 5-node undirected motifs. Our methods provide unbiased estimators of motif frequencies, and we derive simple and exact formulas for the variances of the estimators. Moreover, our methods are designed to fit vertex centric programming models, so they can be easily applied to current graph computing systems such as Pregel and GraphLab. We conduct experiments on a variety of real-world datasets, and experimental results show that our methods are several orders of magnitude faster than the state-of-the-art methods under the same estimation errors.

1. INTRODUCTION

Design tools for counting the frequencies of the appearance of 3-, 4-, and 5-node connected subgraph patterns (i.e., motifs, also known as graphlets) in a graph is important for understanding and exploring networks such as online social networks and computer networks. For example, medium-size networks Slashdot [15] and Epinions [24] have $10^5$ nodes and $10^6$ edges but have more than $10^{10}$ 4-node connected and induced subgraphs (CISes) [29]. To address this problem, cheaper methods such as sampling can be used rather than the brute-force enumeration method. Unfortunately, existing methods of estimating motif concentrations [13,11] cannot be used to estimate motif frequencies, which are more fundamental than motif concentrations.

Despite recent efforts to count triangles [27,22,10,1], little attention has been given to developing scalable tools that can be used to characterize 4- and 5-node motifs. Jha et al. [11] develop sampling methods to estimate 4-node undirected motifs frequencies. In our experiment we observe that their methods do not bound the estimation error tightly, so they significantly over-estimate the sampling budget required to achieve a certain accuracy. Meanwhile, their methods cannot be easily extended to characterize 5-node undirected motifs. Moreover, their methods use an edge-centric program model, so it is difficult to implement them on current graph computing systems such as Pregel [29], GraphLab [19], and GraphChi [16]. In this paper, we propose new methods to estimate the frequencies of 4- and 5-node motifs. Our contributions are summarized as: 1) Our methods of sampling 4- and 5-node motifs are computational efficient and scalable. Meanwhile, they can be easily implemented via vertex centric programming models, which are required by most current graph computing systems. 2) To validate our methods, we perform an in-depth analysis. We find that our methods provide unbiased estimators of motif frequencies. To the best of our knowledge, we are the first to derive simple and exact formulas for the variances of the estimators, which is critical for determining a proper sampling budget in practice. Moreover, we conduct experiments on a variety of publicly available datasets, and experimental results show that our methods significantly outperform the state-of-the-art methods.

The rest of this paper is organized as follows. The problem formulation is presented in Section 2. Section 3 introduces preliminaries used in this paper. Section 4 presents our 4- and 5-node motif sampling methods. The performance evaluation and testing results are presented in Section 6. Section 7 summarizes related work. Concluding remarks then follow.

2. PROBLEM FORMULATION
Let $G = (V, E)$ be the undirected graph of interest, where $V$ and $E$ are the sets of nodes and edges respectively. To formally define 4- and 5-node motif frequencies of $G$, we first introduce some notations. An induced subgraph of $G$, $G' = (V', E')$, is a subgraph whose edges are all in $G$, i.e. $V' \subseteq V$, $E' = \{(u, v) : u,v \in V', (u,v) \in E \}$. We would like to point out that if we do not say “induced” in this paper, we mean that a subgraph is not necessarily induced. Fig. 1(a) shows all 4-node motifs $M_1^{(4)}, \ldots, M_6^{(4)}$ of any undirected network. Denote $C_i^{(4)}$ as the set of 4-node CISes in $G$ isomorphic to motif $M_i^{(4)}$, and then the motif frequency of $M_i^{(4)}$ is defined as $n_i = |C_i^{(4)}|$, $1 \leq i \leq 6$. Fig. 1(b) shows all 5-node motifs $M_1^{(5)}, \ldots, M_{21}^{(5)}$ of any undirected network. Denote $C_i^{(5)}$ as...
the set of 5-node CISes in $G$ isomorphic to motif $M_i^{(5)}$, and then the motif frequency of $M_i^{(5)}$ is defined as $\eta_i = |C_i^{(5)}|$, $1 \leq i \leq 21$. In this paper, we aim to develop computational methods to estimate all theorems in this paper in Appendix. We used throughout the paper in Table 1 and we present the proofs of these estimates, we can obtain a more accurate unbiased estimate of $\hat{c}$ of $c$ by solving

$$\min_{\sum_{i=1}^n \alpha_i = 1} \text{Var} (\hat{c}) = \text{Var} \left( \sum_{i=1}^n \alpha_i (c_i) \right).$$

We can easily obtain the optimal $\text{Var} (\hat{c}) = \frac{1}{\sum_{j=1}^n \var_{wor}(c_j)}$ when $\alpha_i = \frac{\var_{wor}(c_i)}{\sum_{j=1}^n \var_{wor}(c_j)}$. We can also estimate the confidence interval of $\hat{c}$ by the Central Limit Theorem. That is, as $n \to +\infty$, for any $\beta > 0$, we have

$$\Pr \left( |\hat{c} - c| \geq \varepsilon \sqrt{\text{Var}(\hat{c})} \right) \to \frac{1}{\sqrt{2\pi}} \int_{\varepsilon}^{+\infty} e^{-t^2/2} \, dt \approx e^{-\varepsilon^2/2}. $$

3.2 3-Path Sampling Methods

To describe the state-of-the-art 4-node motif sampling methods: 3-path sampling and centered 3-path sampling [11], we first introduce some notations. Let $N_v$ be the set of neighbors of a node $v \in V$ in $G$. Denote the degree of $v$ as $d_v$, which is defined as the number of neighbors of $v$ in $G$, i.e., $d_v = |N_v|$. Let $>_{\text{total}}$ be a total order on all of the nodes in $V$, which can be easily defined and obtained. For example, suppose we order all nodes based on their degrees and node IDs, and we define $u \succ v$ if $d_u > d_v$ or, if $d_u = d_v$ while the node ID of $u$ is larger than that of $v$. Let $N_{u,v}$ denote the set of $u$’s neighbors with order larger than $v$, i.e.,

$$N_{u,v} = \{ x : x \in N_u, \text{ and } x > v \}. $$

Denote $d_{u,v} = |N_{u,v}|$. To sample a 4-node CIS, the 3-PATH sampling method mainly consists of five steps: 1) Sample an edge $e = (u, v)$ from $E$ according to the distribution

$$\{\pi_{(u,v)} = \frac{(d_u - 1)(d_v - 1)}{\sum_{(u',v') \in E} (d_u' - 1)(d_v' - 1)} : (u, v) \in E\},$$

i.e., the probability of sampling an edge $(u, v) \in E$ is $\pi_{(u,v)}$; 2) Sample a node $w$ from $N_u - \{u\}$ uniformly at random; 3) Sample a node $r$ from $N_u - \{v\}$ uniformly at random; 4) Retrieve the CIS $s$ including nodes $v, u, w,$ and $r$. Note that $s$ might be a 3-node CIS when $r = w$.

Compared to 3-path sampling, centered 3-path sampling is tailored to estimate the frequencies of 4-node motifs $M_3^{(4)}, M_4^{(4)}$, and $M_5^{(4)}$, which are usually not frequently appeared in many real networks. To sample a 4-node CIS, the centered 3-PATH sampling method mainly consists of five steps: 1) Sample an edge $e = (u, v)$ from $E$ according to the distribution

$$\{\pi_{(u,v)} = \frac{d_{u,v}d_{v,u}}{\sum_{(u',v') \in E} d_{u',v'}d_{v',u'} : (u', v') \in E}\};$$

2) Sample a node $w$ from $N_{u,v}$ at random; 3) Sample a node $r$ from $N_{u,v}$ at random; 4) Retrieve the CIS $s$ including nodes $v, u, w,$ and $r$. Similarly, $s$ might be a 3-node CIS.

3.3 Vertex-Centric Programming Model

Vertex-centric programming models require users to express their algorithms by “thinking like a vertex”. Each node contains information about itself and all its immediate neighbors, and the algorithms’ operations are executed at the level of a single node. For
example, the operations of a node in Pregel involve receiving messages from other nodes, updating the state of itself and its edges, and sending messages to other nodes. Vertex-centric models are very easy to program and have been widely used for many graph mining and machine learning algorithms.

4. SAMPLING 4-NODE MOTIFS

In this section, we introduce our sampling methods: MOSS-4 and MOSS-4Min. MOSS-4 is used to estimate all 4-node motifs’ frequencies. We observe that MOSS-4 might exhibit large errors for characterizing rare motifs (i.e., motifs with low frequencies) for a small sampling budget. In addition to MOSS-4, we also develop a method MOSS-4Min to further reduce the errors for characterizing rare motifs.

4.1 MOSS-4

4.1.1 Sampling

Denote by \( \Gamma_v = \{(d_x - 1) \sum_{x \in N_v} (d_x - 1)\} \). We assign a weight \( \gamma_v \) to each node \( v \in V \). Define \( \Gamma = \sum_{v \in V} \gamma_v \) and \( \pi_v = \frac{\gamma_v}{\Gamma} \). Our method of sampling a 4-node CIS mainly consists of five steps: 1) Sample a node \( v \) from \( V \) according to the distribution \( \pi = \{\pi_v : v \in V\} \); 2) Sample a random node \( u \) from \( N_v \) according to the distribution \( \sigma^{(v)} = \{\sigma_u^{(v)} : u \in N_v\} \), where \( \sigma_u^{(v)} \) is defined as

\[ \sigma_u^{(v)} = \frac{d_u - 1}{\sum_{x \in N_v} (d_x - 1)}, \quad u \in N_v; \]

3) Sample a node \( w \) from \( N_u - \{u\} \) uniformly at random; 4) Sample a node \( r \) from \( N_u - \{v\} \) uniformly at random; 5) Retrieve the CIS \( s \) including nodes \( v, u, w, \) and \( r \). We set the sampling budget as \( K \), i.e., we run the above method \( K \) times to obtain \( K \) CISs \( s_1, \ldots, s_K \). The pseudo-code of MOSS-4 is shown in Algorithm 1. In Algorithm 1, function WeightRandomVertex(V, \( \pi \)) returns a node sampled from \( V \) according to the distribution \( \pi = \{\pi_v : v \in V\} \), function RandomVertex(X) returns a node sampled from \( X \) at random, and function CIS\{(v, u, w, r)\} returns the CIS with the node set \{v, u, w, r\} in \( G \).

4.1.2 Estimator

Let \( \varphi_i^{(4)} \), \( 1 \leq i \leq 6 \), be the number of subgraphs in motif \( M_i^{(4)} \) that are isomorphic to motif \( M_i^{(4)} \). We can easily compute \( \varphi_1^{(4)} = 1, \varphi_2^{(4)} = 0, \varphi_3^{(4)} = 4, \varphi_4^{(4)} = 2, \varphi_5^{(4)} = 6, \) and \( \varphi_6^{(4)} = 12 \). To remove the error introduced by sampling, we analyze the bias of MOSS-4 as follows:

**Theorem 2.** When the sampling budget \( K = 1 \), MOSS-4 samples a CIS \( s \in C_i^{(4)} \) with probability \( p_i = \frac{2\varphi_i^{(4)}}{K}, 1 \leq i \leq 6 \).

Algorithm 1: The pseudo-code of MOSS-4.

```pseudo
/* K is the sampling budget. */
input : G = (V, E) and K.
output : \( \hat{n}_i, 1 \leq i \leq 6 \).
for i in \{1, 3, 4, 5, 6\} do
    \( \tilde{n}_i \leftarrow 0; \)
end
for k in [1, K] do
    v \leftarrow WeightRandomVertex(V, \pi);
    u \leftarrow WeightRandomVertex(N_v, \sigma^{(v)});
    w \leftarrow RandomVertex(N_u - \{v\});
    r \leftarrow RandomVertex(N_u - \{v\});
    s_k \leftarrow CIS\{(v, u, w, r)\};
    if r \neq u and r \neq w then
        i \leftarrow M_i^{(4)}(s_k);
        \( \hat{n}_i \leftarrow \hat{n}_i + \frac{1}{K}; \)
    end
end
\( \hat{n}_2 \leftarrow \Lambda_3 - \hat{n}_4 - 2\hat{n}_5 - 4\hat{n}_6; \)
```

We let \( M_i^{(4)}(s_k) \) be the 4-node motif class ID of \( s_k \) when \( s_k \) is a 4-node CIS, and -1 otherwise (i.e., \( s_k \) is a triangle). Let \( \chi(X) \) denote the indicator function that equals one when predicate \( X \) is true, and zero otherwise. Denote \( m_i = \sum_{k=1}^K 1(M_i^{(4)}(s_k) = i) \). For \( i \in \{1, 3, 4, 5, 6\} \), \( p_i \) is larger than zero and we estimate \( n_i \) as

\[ \hat{n}_i = \frac{m_i}{K p_i}, \quad i \in \{1, 3, 4, 5, 6\}. \]
Let $\Lambda_3 = \sum_{v \in V} (\frac{d_v}{3})^2$. Then, the number of all 4-node subgraphs (not necessarily induced) in $G$ isomorphic to motif $M_2^{(4)}$ is $\Lambda_3$. Let $\varphi_i^{(2)}$, $1 \leq i \leq 6$, be the number of subgraphs in motif $M_2^{(4)}$ that are isomorphic to motif $M_2^{(2)}$. We have $\varphi_1^{(2)} = 0$, $\varphi_2^{(2)} = 1$, $\varphi_3^{(2)} = 0$, $\varphi_4^{(2)} = 1$, $\varphi_5^{(2)} = 2$, and $\varphi_6^{(2)} = 4$. We can easily find that

$$\Lambda_3 = \sum_{i=1}^{6} \varphi_i^{(2)} n_i = n_2 + n_4 + 2n_5 + 4n_6. \quad (2)$$

Thus, we estimate $n_2$ as

$$\hat{n}_2 = \Lambda_3 - \hat{n}_4 - 2\hat{n}_5 - 4\hat{n}_6.$$ 

**Theorem 3.** $\hat{n}_4$ is an unbiased estimator of $n_i$, $1 \leq i \leq 6$.

The variance of $\hat{n}_4$ is

$$\text{Var}(\hat{n}_4) = \frac{n_4}{K} \left( \frac{1}{p_4} - 1 \right), \quad i \in \{1, 3, 4, 5, 6\}.$$ 

The variance of $\hat{n}_5$ is computed as

$$\text{Var}(\hat{n}_5) = \frac{1}{K} \left( \frac{n_4}{p_4} + \frac{4n_5}{p_w} + \frac{16n_6}{p_6} - \left( n_4 + 2n_5 + 4n_6 \right)^2 \right).$$

From Theorem 1 we can easily compute a sampling budget $K$ that can guarantee $P(\hat{n}_4 - n_4 > \varepsilon n_4) < \delta$ for any $\varepsilon > 0$ and $0 < \delta < 1, i = 1, \ldots, 6$.

### 4.1.3 Computational Complexity

**Initialization:** For each node $v$, we store its degree $d_v$ and use a list to store its neighbors $N_v$. Therefore, it requires $O(d_v)$ operations to compute $\Gamma_v$, and the computational complexity of processing all nodes is $O(|E|)$.

**WeightRandomVertex($V, \pi$):** We use a list $V[1, \ldots, |V|]$ to store the nodes in $V$. We store an array $ACC_{\Gamma}[1, \ldots, |V|]$ in memory, where $ACC_{\Gamma}[i]$ is defined as $ACC_{\Gamma}[i] = \sum_{j=1}^{i} \Gamma_{V[j]}$, $1 \leq i \leq |V|$. Clearly, $ACC_{\Gamma}[|V|] = \Gamma$. Let $ACC_{\Gamma}[0] = 0$. Then, WeightRandomVertex($V, \pi$) can be easily achieved by the following three steps:

- Step 1: Select a number $\text{rnd}$ from $\{1, \ldots, \Gamma\}$ at random;
- Step 2: Find $i$ satisfying $ACC_{\Gamma}[i-1] < \text{rnd} \leq ACC_{\Gamma}[i]$,
- Step 3: Return $V[i]$.

Its computational complexity is $O(\log |V|)$.

**WeightRandomVertex($N_v, \sigma^{(v)}$):** We use a list $N_v[1, \ldots, d_v]$ to store the neighbors of $v$. We store an array $ACC_{\sigma^{(v)}[1, \ldots, d_v]}$ in memory, where $ACC_{\sigma^{(v)}[i]}$ is defined as $ACC_{\sigma^{(v)}[i]} = \sum_{j=1}^{i} (d_{N_v[j]} - 1)$, $1 \leq i \leq d_v$. Let $ACC_{\sigma^{(v)}[0]} = 0$. Then, WeightRandomVertex($N_v, \sigma^{(v)}$) can be easily achieved by the following three steps:

- Step 1: Select a number $\text{rnd}$ from $\{1, \ldots, ACC_{\sigma^{(v)}[d_v]}\}$ at random;
- Step 2: Find $i$ satisfying $ACC_{\sigma^{(v)}[i-1]} < \text{rnd} \leq ACC_{\sigma^{(v)}[i]}$,
- Step 3: Return $N_v[i]$.

Its computational complexity is $O(\log d_v)$.

**RandomVertex($N_v \setminus \{u\}$):** Let $POS_{v,u}$ denote the index of $u$ in the list $N_v[1, \ldots, d_v]$, i.e., $N_v[POS_{v,u}] = u$. Then, function RandomVertex($N_v \setminus \{u\}$) can be achieved by the following steps:

- Step 1: Select a number $\text{rnd}$ from $\{1, \ldots, d_v\} \setminus \{POS_{v,u}\}$ at random;
- Step 2: Return $N_v[\text{rnd}]$.

Its computational complexity is $O(1)$.

In summary, the complexity of MOSS-4 sampling $K$ CISes is $O(|E| + K \log |V|)$.

### 4.2 MOSS-4Min

#### 4.2.1 Sampling

From the above derived formulas of the variances of MOSS-4, we can see that MOSS-4 might exhibit larger errors for 4-node motifs with lower frequencies when allocating a small sampling budget $K$. To solve this problem, we develop a better method MOSS-4Min to further reduce the errors for estimating the frequencies of 4-node motifs $M_2^{(4)}, M_3^{(4)}$, and $M_4^{(4)}$.

Let $\Gamma_v = \sum_{e \in E} d_{N_v} v, v \in V$. MOSS-4Min assigns a weight $\Gamma_v$ to each node $v \in V$. Define $\hat{\Gamma} = \sum_{v \in V} \Gamma_v$ and $\hat{\pi}_v = \frac{\Gamma_v}{\hat{\Gamma}}$. MOSS-4Min mainly consists of five steps: 1) Sample a node $v$ from $V$ according to the distribution $\pi = \{\pi_v : v \in E\}$. 2) Sample a node $u$ from $N_v$ according to the distribution $\hat{\sigma}^{(v)} = \{\hat{\sigma}_u^{(v)} : u \in N_v\}$, where $\hat{\sigma}_u^{(v)}$ is defined as

$$\hat{\sigma}_u^{(v)} = \frac{d_u d_{v,N_u}}{\Gamma_v}, \quad u \in N_v; \quad (3)$$

3) Sample a node $w$ from $N_{u,v}$ at random; 4) Sample a node $r$ from $N_{u,v}$ at random; 5) Retrieve the CISs including nodes $v, u, w,$ and $r$. We set the sampling budget as $K$ to obtain $K$ CISes $s_1, \ldots, s_K$.

#### 4.2.2 Estimator

Algorithm 2: The pseudo-code of MOSS-4Min.

```plaintext
Algorithm 2: The pseudo-code of MOSS-4Min.

\textbf{input:} $G = (V, E)$ and $K$.
\textbf{output:} $\hat{n}_i, i \in \{3, 5, 6\}$.
\textbf{for} $k \in [1, K]$ \textbf{do}
\textbf{for} $v \in \text{WeightRandomVertex}(V, \pi)$;
\textbf{for} $u \in \text{WeightRandomVertex}(N_v, \hat{\sigma}^{(v)})$;
\textbf{for} $w \in \text{RandomVertex}(N_{v,u})$;
\textbf{for} $r \in \text{RandomVertex}(N_{u,v})$;
\textbf{for} $s_k \in \text{CIS}(v, u, w, r)$;
\textbf{if} $r \neq u$ and $r \neq w$ \textbf{then}
\textbf{for} $i \in \{3, 5, 6\}$ \textbf{do}
\textbf{if} $i = 3$ \textbf{then}
\textbf{end}
\textbf{end}
\textbf{end}
```

**Theorem 4.** When the sampling budget $K = 1$, MOSS-4Min samples CISes $s \in C_4^{(4)}$, $s \in C_3^{(5)}$, and $s \in C_6^{(4)}$ with probabilities $\tilde{p}_3 = 2\Gamma^{-1}$, $\tilde{p}_5 = 2\Gamma^{-1}$, and $\tilde{p}_6 = 6\Gamma^{-1}$ respectively.
We estimate $n_3$, $n_5$, and $n_6$ as

$$\tilde{n}_i = \sum_{k=1}^{\tilde{K}} \frac{m_i}{K \tilde{p}_i}, \quad i = 3, 5, 6,$$

where $m_i = \sum_{k=1}^{K} 1(M^{(i)}(s_k) = i)$. The variances of $n_3$, $n_5$, and $n_6$ are given in the following theorem. We omit the proof, which is analogous to that of Theorem 3.

**Theorem 5.** $\tilde{n}_i$ is an unbiased estimator of $n_i$, $i = 3, 5, 6$. Its variance is

$$\text{Var}(\tilde{n}_i) = \frac{n_i}{K} \left(1 - \frac{1}{\tilde{p}_i} - n_i\right), \quad i = 3, 5, 6.$$

From Theorems 1, 2, and 5, we can easily obtain a more accurate estimator of $n_i$ by combining $\hat{n}_i$ and $\tilde{n}_i$, $i = 3, 5, 6$.

### 4.2.3 Computational Complexity

We easily extend methods in Section 4.1.3 to design functions WeightRandomVertex($V, \tilde{\pi}$) and WeightRandomVertex($N_v, \sigma^{(v)}$) in Algorithm 2. The computational complexity of MOSS-4min sampling $K$ CISes is $O(|E| + K \log |V|)$.

### 4.3 Vertex-Centric Programming Models

In this subsection, we show MOSS-4 and MOSS-4Min can be easily implemented via vertex-centric programming models.

#### 4.3.1 Vertex-Centric Programming Model of MOSS-4 Sampling Method

First, we sample $K$ nodes in $V$ according to $\pi$. Let $k_v$ denote the number of times a node $v \in V$ sampled. Thus, $\sum_{v \in V} k_v = K$. For each node $v$, we set $k_v$ as its node value, and then repeat the set of four following operations $k_v$ times

1. $u \leftarrow \text{WeightRandomVertex}(N_u, \sigma^{(u)})$,
2. $w \leftarrow \text{RandomVertex}(N_v)$,
   - Update($A$) and then MSG($v, u, w, *, A$) $\rightarrow u$,
   - When a node $u$ receives a message like $(v, *, w, *, A)$, do $r \leftarrow \text{RandomVertex}(N_u)$,
     - Update($A$) and then MSG($v, u, w, *, A$) $\rightarrow r$.

where $A$ is the adjacent matrix of the CIS consisting of nodes $v$, $u$, $w$, and $r$, which are the variables in the Algorithm 2, i.e., the nodes sampled at the 1-st, 2-nd, 3-rd, and 4-th steps respectively. Note that here $r$ and some entries in $A$ are unknown. Function Update($A$) is used to get the values of unknown entries in $A$ based on the edges of the current node $v$. Function MSG($v, *, w, *, A$) $\rightarrow u$ generates a message $(v, *, w, *, A)$, and sends the message to $u$, which is a neighbor of $v$.

We process the messages that a node receives as follows:

- When a node $u$ receives a message like $(v, *, w, *, A)$, we first Update($A$). From $A$ we then have all the edges between $v$, $u$, $w$, and $r$. Last, we set $m_i \leftarrow m_i + 1$, where $i$ is the motif class of the CIS consisting of $v$, $u$, $w$, and $r$.

#### 4.3.2 Vertex-Centric Programming Model of MOSS-4Min Sampling Method

Similar to MOSS-4, we sample $K$ nodes in $V$ according to $\tilde{\pi}$. Let $\tilde{k}_v$ denote the number of times a node $v \in V$ sampled. Thus, $\sum_{v \in V} \tilde{k}_v = \tilde{K}$. For each node $v$, we set $\tilde{k}_v$ as its node value, and then repeat the set of four following operations $\tilde{k}_v$ times

$$u \leftarrow \text{WeightRandomVertex}(N_u, \tilde{\sigma}^{(v)})$$

$$w \leftarrow \text{RandomVertex}(N_v),$$

Update($A$) and then MSG($v, u, w, *, A$) $\rightarrow u$.

We process the messages that a node receives as follows:

- When a node $u$ receives a message like $(v, *, w, *, A)$, do $r \leftarrow \text{RandomVertex}(N_u)$,

- Update($A$) and then MSG($v, u, w, *, A$) $\rightarrow r$.

4.4 Relationship to 3-Path Sampling and Centered 3-Path Sampling

MOSS-4 and MOSS-4Min can be viewed as the vertex-centric versions of the 3-path and centered 3-path sampling methods respectively. Suppose we use 4 bytes to store a node ID and its weight $\Gamma_v$. The 3-path and centered 3-path sampling methods require $8|E| + 4d_{max}$ bytes of memory, but MOSS-4 and MOSS-4MIN need only $4(|V| + d_{max})$ bytes, which is orders of magnitude smaller than $8|E| + 4d_{max}$ for many real-world large networks. Therefore, MOSS-4 and MOSS-4Min are suit for disk-based graph computing systems such as GraphChi and VENUS [5], which aim to analyze big graphs when the graphs of interest cannot be fitted into memory. Moreover, MOSS-4 and MOSS-4Min can be easily implemented in distributed vertex-centric graph computing systems such as Pregel and GraphLab. Meanwhile, we would like to point out we give the closed-form formulas for the variances of MOSS-4 and MOSS-4MIN. They are critical to evaluate the error of an estimate and determine a proper sampling budget in order to guarantee certain accuracy. Moreover, they can also help us to make the right sampling strategies in advance. An example is given in the following subsection.

4.5 Compare MOSS-4 and MOSS-4MIN

From Theorems 3 and 5 when $K = \tilde{K}$, we have

$$\frac{\text{Var}(\tilde{n}_i)}{\text{Var}(n_i)} = \frac{1/\tilde{p}_i - n_i}{1/p_i - n_i} \approx \frac{\tilde{p}_i}{p_i}, \quad i = 3, 5, 6,$$

where $\tilde{p}_i = \frac{i}{\tilde{d}_i}$, $p_i = \frac{i}{d_i}$, and $\frac{\tilde{p}_i}{p_i} = \frac{\tilde{d}_i}{d_i}$. Thus, the value of $\frac{\tilde{p}_i}{p_i}$ helps us to determine whether it is necessary to apply MOSS-4Min to further reduce the errors of estimating $n_3$, $n_5$, and $n_6$. For example, the graph ca-GrQc [17] has $\frac{\tilde{d}_i}{d_i} = 5.5$. In our experiments we observe that MOSS-4MIN slightly improves the accuracy of MOSS-4 for estimating $n_3$ and $n_6$ of ca-GrQc, and exhibits a larger error than MOSS-4 for estimating $n_5$ of ca-GrQc.

5. SAMPLING 5-NODE MOTIFS

5.1 MOSS-5

MOSS-5, our method of estimating frequency of all 5-node motifs, consists of two sub-methods: T-5 and Path-5. We develop T-5 to sample 5-node CISes that include at least one subgraph isomorphic to $M_5^{(5)}$. Similarly, Path-5 is developed to sample 5-node CISes that include at least one subgraph isomorphic to $M_5^{(5)}$. Finally, we propose a method to estimate the frequency of all 5-node motifs based on sample CISes given by T-5 and Path-5.
### 5.1.1 T-5 Sampling Method

The pseudo-code of T-5 is shown in Algorithm 3. Let \( \Gamma_v^{(1)} = (d_v - 1)(d_v - 2) \sum_{x \in N_v} (d_x - 1), \ v \in V. \)

We assign a weight \( \Gamma_v^{(1)} \) to each node \( v \in V. \) Define \( \Gamma_v^{(1)} = \sum_{v \in V} \Gamma_v^{(1)} \) and \( \rho_v^{(1)} = \frac{\Gamma_v^{(1)}}{\Gamma_v^{(5)}}. \) To sample a 5-node CIS, T-5 mainly consists of five steps: 1) Sample a node \( v \) from \( V \) according to the distribution \( \rho_v^{(1)} = \{ \rho_v^{(1)} : v \in V \}; \) 2) Sample a node \( u \) of \( N_v \) according to the distribution \( \sigma_v^{(u)} = \{ \sigma_v^{(u)} : u \in N_v \}, \) where \( \sigma_v^{(u)} \) is defined the same as in 1; 3) Sample two different nodes \( w \) and \( r \) from \( N_u \setminus \{u\} \) at random; 4) Sample a node \( t \) from \( N_v \setminus \{v\} \) uniformly at random; 5) Retrieve the CIS \( s \) including nodes \( v, u, w, r \) and \( t. \) We run the above method \( K_1 \) times to obtain \( K_1 \) CISEs \( s^{(1)}, \ldots, s^{(K_1)}. \)

**Algorithm 3**: The pseudo-code of T-5.

**input**: \( G = (V, E) \) and \( K_1. \)

**output**: \( \hat{\eta}_i^{(1)}. \)

for \( i \in \Omega_1 \) do

\[
\hat{\eta}_i^{(1)} \leftarrow 0;
\]

end

for \( k \in [1, K_1] \) do

\[
v \leftarrow \text{WeightRandomVertex}(V, \rho_v^{(1)});
\]

\[
u \leftarrow \text{WeightRandomVertex}(N_v, \sigma_v^{(u)});
\]

\[
w \leftarrow \text{RandomVertex}(N_u \setminus \{u\});
\]

\[
r \leftarrow \text{RandomVertex}(N_v \setminus \{u, w\});
\]

\[
t \leftarrow \text{RandomVertex}(N_v \setminus \{v\});
\]

\[
\hat{s}_k^{(1)} \leftarrow \text{CIS}(v, u, w, r, t);
\]

if \( t \neq w \) and \( t \neq r \) then

\[
i \leftarrow M^{(5)}(s_k^{(1)});
\]

\[
\hat{\eta}_i^{(1)} \leftarrow \hat{\eta}_i^{(1)} + \frac{1}{K_1p_i^{(1)}};
\]

end

end

Let \( \phi_i^{(1)}, 1 \leq i \leq 21, \) be the number of subgraphs in motif \( M_i^{(5)} \) that are isomorphic to motif \( M_5^{(5)}. \) The value of \( \phi_i^{(1)} \) is given in Table 2. The following theorem shows the sampling bias of the 5-node T-sampling method.

**Theorem 6.** When the sampling budget \( K_1 = 1, \) T-5 samples a CIS \( s \in C_i^{(5)} \) with probability \( p_i^{(1)} = \frac{2^{\phi_i^{(1)}}}{\Gamma_v^{(1)}}, 1 \leq i \leq 21. \)

We let \( M^{(5)}(s) \) be the 5-node motif class ID of \( s \) when \( s \) is a 5-node CIS, and -1 otherwise. Denote \( \Gamma_i^{(1)} = \sum_{k=1}^{K_1} M_i^{(5)}(s_k^{(1)}) = i. \) Let \( \Omega_1 = \{ j : \phi_j^{(1)} > 0 \}. \) For \( i \in \Omega_1, \) \( p_i^{(1)} \) is larger than zero and we then estimate \( \eta_i \) as

\[
\hat{\eta}_i^{(1)} = \frac{m_i^{(1)}}{K_1p_i^{(1)}}.
\]

**Theorem 7.** For \( i \in \Omega_1, \) \( \hat{\eta}_i^{(1)} \) is an unbiased estimator of \( \eta_i \) and its variance of \( \hat{\eta}_i^{(1)} \) is

\[
\text{Var} \left( \hat{\eta}_i^{(1)} \right) = \frac{\eta_i}{K_1} \left( \frac{1}{p_i^{(1)}} - \eta_i \right).
\]

### 5.1.2 Path-5 Sampling Method

The pseudo-code of Path-5 is shown in Algorithm 4. Let \( \Gamma_v^{(2)} = \sum_{v \in V} \Gamma_v^{(2)} \) and \( \rho_v^{(2)} = \frac{\Gamma_v^{(2)}}{\Gamma_v^{(5)}}. \) To sample a 5-node CIS, Path-5 mainly consists of six steps: 1) Sample a node \( v \) from \( V \) according to the distribution \( \rho_v^{(2)} = \{ \rho_v^{(2)} : v \in V \}; \) 2) Sample a node \( u \) from \( N_v \) according to the distribution \( \nu_v^{(u)} = \{ \nu_v^{(u)} : u \in N_v \}, \) where \( \sum_{u \in N_v} \nu_v^{(u)} = 1 \) and \( \nu_v^{(u)} \) is defined as

\[
\nu_v^{(u)} = \frac{(d_u - 1)(\sum_{y \in N_u \setminus \{u\}} (d_y - 1))}{\Gamma_v^{(2)}}, \ u \in N_v;
\]

3) Sample a node \( w \) from \( N_v \setminus \{u\} \) according to the distribution \( \nu_v^{(w,u)} = \{ \nu_v^{(w,u)} : w \in N_v \setminus \{u\} \}, \) where \( \sum_{w \in N_u \setminus \{u\}} \nu_v^{(w,u)} = 1 \) and \( \nu_v^{(w,u)} \) is defined as

\[
\nu_v^{(w,u)} = \frac{d_w - 1}{\sum_{y \in N_u \setminus \{u\}} (d_y - 1)}, \ w \in N_v \setminus \{u\};
\]

4) Sample a node \( r \) from \( N_u \setminus \{v\} \) uniformly at random; 5) Sample a node \( t \) from \( N_v \setminus \{v\} \) uniformly at random; 6) Retrieve the CIS \( s \) including nodes \( v, u, w, r \) and \( t. \) We run the above method \( K_2 \) times to obtain \( K_2 \) CISEs \( s^{(2)}, \ldots, s^{(K_2)}. \)

**Algorithm 4**: The pseudo-code of Path-5.

**input**: \( G = (V, E) \) and \( K_2. \)

**output**: \( \hat{\eta}_i^{(2)}. \)

for \( i \in \Omega_2 \) do

\[
\hat{\eta}_i^{(2)} \leftarrow 0;
\]

end

for \( k \in [1, K_2] \) do

\[
v \leftarrow \text{WeightRandomVertex}(V, \rho_v^{(2)});
\]

\[
u \leftarrow \text{WeightRandomVertex}(N_v, \nu_v^{(u)});
\]

\[
w \leftarrow \text{WeightRandomVertex}(N_u \setminus \{u\}, \nu_v^{(w,u)});
\]

\[
r \leftarrow \text{RandomVertex}(N_v \setminus \{v\});
\]

\[
t \leftarrow \text{RandomVertex}(N_v \setminus \{v\});
\]

\[
\hat{s}_k^{(2)} \leftarrow \text{CIS}(v, u, w, r, t);
\]

if \( t \neq u \) and \( t \neq r \) then

\[
i \leftarrow M^{(5)}(s_k^{(2)});
\]

\[
\hat{\eta}_i^{(2)} \leftarrow \hat{\eta}_i^{(2)} + \frac{1}{K_2p_i^{(2)}};
\]

end

end

Let \( \phi_i^{(2)}, 1 \leq i \leq 21, \) be the number of subgraphs in motif \( M_i^{(5)} \) that are isomorphic to motif \( M_5^{(5)}. \) The value of \( \phi_i^{(2)} \) is given in Table 2. The following theorem shows the sampling bias of Path-5.

**Theorem 8.** When the sampling budget \( K_2 = 1, \) Path-5 samples a CIS \( s \in C_i^{(5)} \) with probability \( p_i^{(2)} = \frac{2^{\phi_i^{(2)}}}{\Gamma_v^{(2)}}, 1 \leq i \leq 21. \)
Denote \( m_i^{(2)} = \sum_{k=1}^{K_2} 1(M^{(5)}(v_k) = i) \). Let \( \Omega_2 = \{ j : \phi_j^{(2)} > 0 \} \). For \( i \in \Omega_2 \), \( p_i^{(2)} \) is larger than zero and we then estimate \( \eta_i \) as
\[
\hat{\eta}_i^{(2)} = \frac{m_i^{(2)}}{K_2p_i^{(2)}}.
\]

**Theorem 9.** For \( i \in \Omega_2 \), \( \hat{\eta}_i^{(2)} \) is an unbiased estimator of \( \eta_i \) and its variance of \( \hat{\eta}_i^{(2)} \) is
\[
\text{Var}(\hat{\eta}_i^{(2)}) = \frac{\eta_i}{K_2^2} \left( \frac{1}{p_i^{(2)}} - \eta_i \right).
\]

The covariance of \( \hat{\eta}_i^{(2)} \) and \( \hat{\eta}_j^{(2)} \) is
\[
\text{Cov}(\hat{\eta}_i^{(2)}, \hat{\eta}_j^{(2)}) = -\frac{\eta_i \eta_j}{K_2^2}, \quad i \neq j \text{ and } i, j \in \Omega_2.
\]

### 5.1.3 Mix Estimator

We estimate \( \eta_i \) as \( \hat{\eta}_i^{(1)} \) and \( \hat{\eta}_i^{(2)} \) for \( i \in \Omega_1 - \Omega_2 \) and \( i \in \Omega_2 - \Omega_1 \) respectively. When \( i \in \Omega_1 \cap \Omega_2 \), according to Theorem 9, we estimate \( \eta_i \) based on its two estimates \( \hat{\eta}_i^{(1)} \) and \( \hat{\eta}_i^{(2)} \). Formally, we define
\[
\lambda_i^{(1)} = \frac{\text{Var}(\hat{\eta}_i^{(1)})}{\text{Var}(\hat{\eta}_i^{(1)}) + \text{Var}(\hat{\eta}_i^{(2)})}, \quad \lambda_i^{(2)} = \frac{\text{Var}(\hat{\eta}_i^{(2)})}{\text{Var}(\hat{\eta}_i^{(1)}) + \text{Var}(\hat{\eta}_i^{(2)})},
\]
where \( \text{Var}(\hat{\eta}_i^{(1)}) \) and \( \text{Var}(\hat{\eta}_i^{(2)}) \) are given in (11) and (5). For \( i \in \Omega_1 \cup \Omega_2 = \{1, 3, 4, 5, \ldots, 21\} \), finally estimate \( \eta_i \) as
\[
\hat{\eta}_i = \begin{cases} 
\lambda_i^{(1)} \hat{\eta}_i^{(1)} + \lambda_i^{(2)} \hat{\eta}_i^{(2)}, & i \in \Omega_1 \cap \Omega_2, \\
\hat{\eta}_i^{(1)}, & i \in \Omega_1 - \Omega_2, \\
\hat{\eta}_i^{(2)}, & i \in \Omega_2 - \Omega_1.
\end{cases}
\]

We can see that \( \Omega_1 \cup \Omega_2 = \{1, 2, \ldots, 21\} \). Thus, \( \hat{\eta}_i \) can be used to estimate the frequencies of all 5-node motifs except motif \( M_2^{(5)} \). Next, we introduce the method of estimating \( \eta_2 \). Let \( \phi_i^{(3)} \), \( 1 \leq i \leq 21 \), be the number of subgraphs in motif \( M_2^{(5)} \) that are isomorphic to motif \( M_2^{(5)} \). The value of \( \phi_i^{(3)} \) is given in Table 2. Let \( \Lambda_3 = \sum_{v \in V} (d_v) \). Then, the number of all 5-node subgraphs (not necessarily induced) in \( G \) isomorphic to motif \( M_2^{(5)} \) is \( \Lambda_3 \). Let \( \Omega_3 = \{ j : \phi_j^{(3)} > 0 \} \). We observe that
\[
\sum_{i \in \Omega_3} \phi_i^{(3)} \eta_i = \Lambda_3.
\]
Since \( \phi_2^{(3)} = 1 \), we estimate \( \eta_2 \) as
\[
\hat{\eta}_2 = \Lambda_3 - \sum_{i \in \Omega_3^{(3)}} \phi_i^{(3)} \hat{\eta}_i.
\]

### Table 2: Values of \( \phi_1^{(3)} \), \( \phi_2^{(3)} \), and \( \phi_3^{(3)} \).

|  | \( \phi_1^{(3)} \) | \( \phi_2^{(3)} \) | \( \phi_3^{(3)} \) |
|---|---|---|---|
| \( \eta_1 \) | 0 | 0 | 0 |
| \( \eta_2 \) | 0 | 1 | 0 |
| \( \eta_3 \) | 1 | 1 | 0 |

**Theorem 10.** \( \hat{\eta}_i \) is an unbiased estimator of \( \eta_i \), \( 1 \leq i \leq 21 \). For \( i \in \Omega_1 \cup \Omega_2 = \{1, 2, \ldots, 21\} \) and \( i \neq j \), we compute \( \text{Cov}(\hat{\eta}_i, \hat{\eta}_j) = \Phi_i^{(3)} \Phi_j^{(3)} \text{Cov}(\hat{\eta}_i, \hat{\eta}_j) \), where \( \Phi_i^{(3)} = \Omega_3 = \{2\} \).

### 5.1.4 Parameter Setting

From Theorem 10, we can see that the error of \( \hat{\eta}_i \) greatly depends on the sampling budget \( K_1 \) for \( i \in \Omega_1 - \Omega_2 \). In contrast, \( K_2 \) is used to guarantee the accuracy of \( \hat{\eta}_i \), \( i \in \Omega_2 - \Omega_1 \). Thus, \( K_1 \) and \( K_2 \) can be set according to the above observations. In our experiments, we find that \( p_i^{(1)} \) and \( p_i^{(2)} \) have similar values. Therefore, we set \( K_1 = K_2 \) in this paper for simplicity.

### 5.1.5 Computational Complexity

For the T-5 sampling method, we easily extend the methods in Section 4.1.3 to design its functions \( \text{WeightRandomVertex}(V, \rho^{(1)}) \) and \( \text{WeightRandomVertex}(V, \sigma^{(v)}) \) in Algorithm 3. Thus, the computational complexity of T-5 sampling \( K_1 \) CISes is \( O(\|E\| + K_1 \log |V|) \).

For the Path-5 sampling method, we easily extend the methods in Section 4.1.3 to design its functions \( \text{WeightRandomVertex}(V, \rho^{(2)}) \) and \( \text{WeightRandomVertex}(V, \mu^{(v,u)}) \) in Algorithm 4. Next, we present our method of implementing \( \text{WeightRandomVertex}(N_v, \tau^{(v)}) \) in Algorithm 4. As alluded, we use a list \( N_v[1, \ldots, d_v] \) to store the neighbors of \( v \). We store an array \( ACC^{(v)}[1, \ldots, d_v] \) in memory, \( \text{ACC}_v^{(v)}[i] = \sum_{j=1}^{d_v} d_{v,j} - 1 \), \( 1 \leq i \leq d_v \). Let \( \text{ACC}^{(v)}[0] = 0 \). Let \( \text{POS}_v^{(u)} \) be the index of \( u \) in \( N_v[1, \ldots, d_v] \), i.e., \( N_v[\text{POS}_v^{(u)}] = u \). Then, function \( \text{WeightRandomVertex}(N_v - \{u\}, \mu^{(v,u)}) \) can be easily achieved by the following three steps:
• Step 1: Select a number \( r_{\text{nd}} \) from \( \{1, \ldots, ACC_{n, \mu}^{(v)}[d_{v}]\} - \{ACC_{n, \mu}^{(v)}[\text{POS}_{v, u} - 1] + 1, \ldots, ACC_{n, \mu}^{(v)}[\text{POS}_{v, u}]\} \) at random;
• Step 2: Find \( i \) satisfying
  \[ ACC_{n, \mu}^{(v)}[i - 1] < r_{\text{nd}} \leq ACC_{n, \mu}^{(v)}[i], \]
  which can be solved by the binary search algorithm;
• Step 3: Return \( N_{v}[i] \).

Its computational complexity is \( O(\log d_v) \). Therefore, the computational complexity of Path-5 sampling \( K_2 \) CISes is \( O([E] + K_2 \log |V|) \).

5.2 Vertex-Centric Programming Models

In this subsection, we show MOSS-5 can be easily implemented in a vertex-centric programming model.

5.2.1 Vertex-Centric Programming Model of T-5

We sample \( K_1 \) nodes in \( V \) according to \( \rho^{(3)} \). Let \( k^{(3)}_v \) denote the number of times a node \( v \in V \) sampled. Thus, \( \sum_{v \in V} k^{(3)}_v = K_1 \).

For each node \( v \), we set \( k^{(3)}_v \) as its node value, and then repeat the set of five following operations \( k^{(3)}_v \) times

\[
\begin{align*}
  u &\leftarrow \text{WeightRandomVertex}(N_v, \sigma^{(v)}), \\
  w &\leftarrow \text{RandomVertex}(N_v - \{u\}), \\
  r &\leftarrow \text{RandomVertex}(N_v - \{u, w\}),
\end{align*}
\]

Update(A) and then MSG\((v, u, w, r, *, A) \rightarrow u\),

where \( A \) is the adjacent matrix of the CIS consisting of nodes \( v, u, w, r, \) and \( t \), which are the variables in Algorithm\(^3\) i.e., the nodes sampled at the 1-st, 2-nd, 3-rd, 4-th, and 5-th steps respectively. Note that here \( t \) and some entries in \( A \) are unknown.

We process the messages that a node receives as follows:

• When a node \( u \) receives a message like \((v, *, w, *, A)\), do
  \[
  t \leftarrow \text{RandomVertex}(N_u - \{v\}),
  \]

  Update(A) and then MSG\((v, u, w, r, *, A) \rightarrow t\).

• When a node \( t \) receives a message like \((v, u, w, r, *, A)\), do
  Update(A) and then MSG\((v, u, w, r, t, A) \rightarrow w\).

We send MSG\((v, u, w, r, t, A) \rightarrow w\) to determine whether there exists an edge between \( w \) and \( r \).

• When a node \( w \) receives a message like \((v, u, w, r, t, A)\), we first Update(A) and then set \( m_i^{(2)} \leftarrow m_i^{(2)} + 1 \), where \( i \) is the 5-node motif class of the CIS consisting of \( v, u, w, r, \) and \( t \).

5.2.2 Vertex-Centric Programming Model of Path-5

We sample \( K_2 \) nodes in \( V \) according to \( \rho^{(2)} \). Let \( k^{(2)}_v \) denote the number of times a node \( v \in V \) sampled. Thus, \( \sum_{v \in V} k^{(2)}_v = K_2 \).

For each node \( v \), we set \( k^{(2)}_v \) as its node value, and then repeat the set of five following operations \( k^{(2)}_v \) times

\[
\begin{align*}
  u &\leftarrow \text{WeightRandomVertex}(N_v, \tau^{(v)}), \\
  w &\leftarrow \text{RandomVertex}(N_v - \{u\}, \mu^{(v,u)}),
\end{align*}
\]

Update(A) and then MSG\((v, *, w, *, *, A) \rightarrow u, \)

where \( A \) is the adjacent matrix of the CIS consisting of nodes \( v, u, w, r, \) and \( t \), which are the variables in Algorithm\(^3\) i.e., the nodes sampled at the 1-st, 2-nd, 3-rd, 4-th, and 5-th steps respectively. Note that here \( t \) and some entries in \( A \) are unknown.

We process the messages that a node receives as follows:

• When a node \( u \) receives a message like \((v, *, w, *, *, A)\), do
  \[
  r \leftarrow \text{RandomVertex}(N_u - \{v\}),
  \]

  Update(A) and then MSG\((v, u, *, r, *, A) \rightarrow w, \)

• When a node \( w \) receives a message like \((v, u, *, r, *, A)\), do
  \[
  t \leftarrow \text{RandomVertex}(N_u - \{v\}),
  \]

  Update(A) and then MSG\((v, u, w, r, *, A) \rightarrow t) \).

• When a node \( t \) receives a message like \((v, u, w, r, *, A)\), do
  Update(A) and then MSG\((v, u, w, r, t, A) \rightarrow r\).

We send MSG\((v, u, w, r, t, A) \rightarrow r\) to determine whether there exists an edge between \( v \) and \( r \).

• When a node \( r \) receives a message like \((v, u, w, r, t, A)\), we first Update(A) and then set \( m_i^{(2)} \leftarrow m_i^{(2)} + 1 \), where \( i \) is the 5-node motif class of the CIS consisting of \( v, u, w, r, \) and \( t \).

6. DATA EVALUATION

6.1 Datasets

We perform our experiments on the following publicly available datasets taken from the Stanford Network Analysis Platform (SNAP\(^4\) which are summarized in Table 3.

| Graph            | nodes | edges | max-degree |
|------------------|-------|-------|------------|
| soc-Epinions1      | 24    | 75,897| 8044       |
| soc-Slashdot08    | 18    | 77,360| 469,180    |
| com-DBLP           | 321   | 317,080|1,049,866  |
| com-Amazon         | 32    | 334,863|925,872     |
| p2p-Gnutella08     | 75    | 6,301 | 20,777     |
| ca-GitQc           | 17    | 5,241 | 14,484     |
| ca-CondMat         | 17    | 23,133| 93,439     |
| ca-HepTh           | 17    | 9,875 | 25,937     |

Table 3: Graph datasets used in our experiments. “edges” refers to the number of edges in the undirected graph generated by discarding edge labels. “max-degree” represents the maximum number of edges incident to a node in the undirected graph.

6.2 Error Metric

We study the normalized root mean square error (NRMSE) to measure the relative error of the motif frequency estimate \( \hat{n}_i \) with respect to its true value \( n_i, i = 1, \ldots, 6 \). NRMSE\((\hat{n}_i)\) is defined as:

\[
\text{NRMSE}(\hat{n}_i) = \frac{\sqrt{\text{MSE}(n_i)}}{n_i}, \quad i = 1, \ldots, 6,
\]

\(^4\)www.snap.stanford.edu
where \( \text{MSE}(\hat{n}_i) \) is defined as
\[
\text{MSE}(\hat{n}_i) = E[(\hat{n}_i - n_i)^2] = \text{Var}(\hat{n}_i) + (E[\hat{n}_i] - n_i)^2.
\]
Moreover, we define a standard error (in short, StdErr) of \( \hat{n}_i \) as
\[
\text{StdErr}(\hat{n}_i) = \frac{\sqrt{\text{Var}(\hat{n}_i)}}{n_i}, \quad i = 1, \ldots, 6.
\]
We can see that \( \text{MSE}(\hat{n}_i) \) decomposes into a sum of the variance and bias of the estimator \( \hat{n}_i \), both quantities are important and need to be as small as possible to achieve good estimation performance. When \( \hat{n}_i \) is an unbiased estimator of \( n_i \), then \( \text{MSE}(\hat{n}_i) = \text{Var}(\hat{n}_i) \) and thus \( \text{NRMSE}(\hat{n}_i) = \sqrt{\text{Var}(\hat{n}_i)/n_i} = \text{StdErr}(\hat{n}_i) \).

In our experiments, we average the estimates and calculate their NRMSEs over 1,000 runs. Similarly, we define NRMSE of \( \hat{M}_i^{(4)} \), i.e., NRMSE of \( \hat{n}_i^{(4)} \) for methods MOSS-4Min and MOSS-5. To validate the effectiveness of our analytical error bounds, we also compute StdErrs of \( \hat{M}_i^{(4)} \), MOSS-4Min, and MOSS-5 based on the derived closed formula of \( \text{Var}(\hat{n}_i) \), \( \hat{\text{Var}}(\hat{n}_i) \), and \( \hat{\text{Var}}(\bar{n}_i) \).

### 6.3 Estimating all 4-node motifs’ frequencies

Figure 2(a) shows the real values of 4-node motif frequencies \( n_i^{(4)} \) for graphs soc-Epinions1, soc-Slashdot08, and com-Amazon, which have \( 2.58 \times 10^{10}, 2.17 \times 10^{10} \), and \( 1.78 \times 10^{8} \) 4-node CISes respectively. We can see that the motif frequencies of \( M_1^{(4)}, M_2^{(4)}, \) and \( M_3^{(4)} \) are several orders of magnitude smaller than that of the other motifs. Fig 2(b) shows the NRMSEs and StdErrs of \( \hat{n}_i^{(4)} \), the estimates of 4-node undirected motifs’ frequencies given by MOSS-4, where we set \( K = 1,000 \). We can see that motifs with high frequencies exhibit larger NRMSEs and StdErrs than motifs with low frequencies. Moreover, we observe that the StdErr of \( \hat{n}_i^{(4)} \) almost equals to the NRMSE of \( \hat{n}_i^{(4)} \), which is consistent to our analysis above. Our derived error formulas indicate that the StdErr of \( \hat{n}_i^{(4)} \) decreases linearly with the sampling budget \( \sqrt{K} \), which helps us to estimate the computational time required to guarantee certain accuracy for the estimate in advance. Fig 2(c) shows the NRMSEs and StdErrs of \( \hat{n}_i^{(4)} \), \( \hat{n}_i^{(4)} \), and \( \hat{n}_i^{(4)} \) given by MOSS-4MIN, where we set \( K = 1,000 \). Similarly, we see that the StdErr of \( \hat{n}_i^{(4)} \) almost equals to the NRMSE of \( \hat{n}_i^{(4)} \), \( i = 3, 5, 6 \). We compute \( \text{NRMSE}(\hat{n}_i^{(4)}) \) to evaluate the performance of MOSS-4Min in comparison with MOSS-4. \( \text{NRMSE}(\hat{n}_i^{(4)}) \) of soc-Slashdot08 is 2.4, 1.9, and 2.3 for \( i = 3, i = 5, \) and \( i = 6 \) respectively. \( \text{NRMSE}(\hat{n}_i^{(4)}) \) of com-Epinions1 is 2.5, 2.0, and 2.4 for \( i = 3, i = 5, \) and \( i = 6 \) respectively. \( \text{NRMSE}(\hat{n}_i^{(4)}) \) of com-Amazon is 1.7, 1.5, and 1.8 for \( i = 3, i = 5, \) and \( i = 6 \) respectively. We can see that MOSS-4Min exhibits a slightly improvement for ca-GrQc, so it is consistent to the analysis in Section 4.5. To guarantee \( P(|\hat{n}_i - n_i| > \varepsilon n_i) < \delta, \) \( i = 1, \ldots, 6 \), we let \( K_i^{1} \) and \( K_i^{0} \) denote the smallest sampling budgets that are determined by our method and the method in [11] respectively. Fig 3 shows the values of \( K_i^{1}/K_i^{0} \), where \( \varepsilon = 0.1 \) and \( \delta = 0.01 \). We can see that the sampling budgets given by the method in [11] are several orders of magnitude larger than our method. It indicates that the method in [11] does not bound the estimation error tightly and so it significantly over-estimates the sampling budget required to achieve a certain accuracy.
6.4 Estimating all 5-node motifs’ frequencies

Figure 4 shows the real values of $\eta_i$, $1 \leq i \leq 21$, for graphs com-Amazon, com-DBLP, p2p-Gnutella08, ca-GrQc, ca-CondMat, and ca-HepTh, which have $8.50 \times 10^9$, $3.34 \times 10^{10}$, $3.92 \times 10^8$, $3.64 \times 10^7$, $3.32 \times 10^6$, and $8.73 \times 10^5$ 5-node CISes respectively. Fig. 5 shows the NRMSEs and StdErrs of $\hat{\eta}_i$, $1 \leq i \leq 21$, where we set $K_1 = 50,000$ and $K_2 = 50,000$. We can see that the StdErrs are very close to the NRMSEs. It indicates that the derived StdErrs can be accurately used to evaluate the error of our estimates given by MOSS-5. To the best of our knowledge, MOSS-5 is the first to provide a simple and accurate formula for analyzing estimation errors of 5-node motif frequencies. The results show that the NRMSEs of all 5-node motifs are smaller than 0.1 for com-Amazon, which is larger than the other graphs studied in this paper. For the other graphs, most 5-node motifs’ NRMSEs are smaller than 0.1. The NRMSE of $\hat{\eta}_1$ is larger than 1 for p2p-Gnutella08, and the NRMSE of $\hat{\eta}_2$ is larger than 1 for ca-GrQc. We observe that p2p-Gnutella08 has only several CISes isomorphic to $M_1^{(5)}$, and p2p-Gnutella08 has no more than 200 CISes isomorphic to $M_2^{(5)}$. It is very challenging to observe and count these rare motifs for sampling based methods. Most previous work focuses on estimating 5-node motif concentrations, which is defined as $\omega_i = \frac{\eta_i}{\sum_{i=1}^{21}\eta_i}$, $i = 1, \ldots, 21$. We run MOSS-5, state-of-the-arts methods Guise [4] and Graft [23] over all above graphs and increase their sampling budgets until the estimation errors of motif concentrations are within 10%. Fig. 6 shows the runtimes of Graft and Guise normalized with respect to the runtimes of MOSS-5. We can see that our method MOSS-5 is 2 to 3 orders of magnitude faster than Graft and Guise.

7. RELATED WORK

In this paper, we study the problem of computing 4- and 5-node motifs’ frequencies for a single large graph, which is much different from the problem of computing the number of subgraph patterns appearing in a large set of graphs studied in [7]. Recently, a lot of efforts has been devoted to design sampling methods for computing a large graph’s motif concentrations [14, 31, 21, 4, 23, 29]. However, these methods fail to compute motif frequencies, which is more fundamental than motif concentrations. Alon et al. [3] propose the color-coding method to reduce the computational cost of counting subgraphs. Color coding reduces the computations by coloring nodes randomly and enumerating only colorful CISes (i.e., CISes that are consisted of nodes with distinct colors), but [12] reveals that the color-coding method is not scalable and is hindered by the sheer number of colorful CISes. [27, 22, 10] develop sampling methods to estimate the number of triangles of static and dynamic graphs. Jha et al. [11] develop sampling methods to estimate 4-node undirected motifs’ frequencies. However their methods are edge centric methods, which cannot be easily applied to current vertex centric graph computing systems such as GraphLab [19] and GraphChi [16]. Moreover, their methods fail to sample and count 5-node motifs.

8. CONCLUSIONS

We develop computationally efficient sampling methods MOSS-4 and MOSS-5 to estimate the frequencies of all 4- and 5-node motifs. Compared MOSS-4, MOSS-4Min is better to characterize rare motifs. All these methods provide unbiased estimators of motif frequencies, and we derive simple and exact formulas for the variances of the estimators. Meanwhile, we conduct experiments on a variety of publicly available datasets, and experimental results show that our methods significantly outperform state-of-the-art methods.
Motif ID $i$
error
StdErr
NRMSE

(a) com-Amazon

(b) soc-DBLP

(c) p2p-Gnutella08

(d) ca-GrQc

(e) ca-CondMat

(f) ca-HepTh

Figure 5: Real values, StdErrs, and NRMSEs of $\hat{\eta}(5)_i$, i.e., the motif frequency estimates of $M_i^{(5)}$, $1 \leq i \leq 21$, where $K_1 = 50,000$ and $K_2 = 50,000$.

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Appendix
Proof of Theorem 2
As shown in Fig. 7 we find that there exist two ways to sample a subgraph isomorphic to motif $M_i^{(4)}$ by MOSS-4. Each one happens with probability $\pi_v \times \sigma_u^{(v)} \times \frac{1}{d_u-1} \times \frac{1}{d_v-1} = \frac{1}{2}$. For a 4-node CIS $s$ isomorphic to motif $M_i^{(4)}$, $s$ has $\varphi^{(1)}$ subgraphs isomorphic to motif $M_i^{(4)}$, $1 \leq i \leq 6$. Thus, there exist $2\varphi^{(1)}$ ways to sample $s$ by MOSS-4, and the probability of MOSS-4 sampling $s$ is $\frac{2\varphi^{(1)}}{4}$.

Figure 7: The ways of MOSS-4 sampling a subgraph $s$ isomorphic to motif $M_i^{(4)}$, where $v_3, u, w,$ and $r$ are the variables in Algorithm 1 i.e., the nodes sampled at the 1-st, 2-nd, 3-rd, and 4-th steps respectively.

Proof of Theorem 3
For $i \in \{1, 3, 4, 5, 6\}$ and $1 \leq k \leq K$, we have

$$P(M_i^{(4)}(s_k) = i) = \sum_{s \in C(s)} P(s_k = s)1(M_i^{(4)}(s) = i) = p_i n_i.$$
$s_1, \ldots, s_K$ are sampled independently, so the random variable $m_i$ follows the binomial distribution with parameters $K$ and $p_i n_i$. Formally, we have

$$P(m_i = x) = \binom{K}{x} (p_i n_i)^x (1 - p_i n_i)^{K-x}, \quad x = 0, 1, \ldots, K.$$  

Then, the expectation and variance of $m_i$ are

$$E(m_i) = K p_i n_i,$$

and

$$\text{Var}(m_i) = K p_i (1 - p_i n_i).$$

Therefore, the expectation and variance of $\hat{n}_i$ are computed as

$$E(\hat{n}_i) = E \left( \frac{m_i}{K p_i} \right) = \frac{E(m_i)}{K} = \frac{n_i}{K}, \quad (8)$$

and

$$\text{Var}(\hat{n}_i) = \text{Var} \left( \frac{m_i}{K p_i} \right) = \frac{\text{Var}(m_i)}{K^2 p_i^2} = \frac{n_i}{K^2} \left( 1 - \frac{1}{p_i} - \frac{1}{n_i} \right). \quad (9)$$

From (8), we compute the expectation of $\hat{n}_2$ as

$$E(\hat{n}_2) = E(A_3 - \hat{n}_4 - 2\hat{n}_5 - 4\hat{n}_6) = A_3 - E(\hat{n}_4) - 2E(\hat{n}_5) - 4E(\hat{n}_6) = A_3 - n_4 - 2n_5 - 4n_6 = n_2.$$  

The last equation holds because of (2). To derive the variance of $\hat{n}_2$, we first compute the covariance of $\hat{n}_i$ and $\hat{n}_j$, where $i \neq j$ and $i, j \in \{1, 3, 4, 5, 6\}$. That is,

$$\text{Cov}(\hat{n}_i, \hat{n}_j) = \text{Cov} \left( \frac{m_i}{K p_i}, \frac{m_j}{K p_j} \right) = \frac{\text{Cov}(\sum_{k=1}^{K} 1(M^{(4)}(s_k) = i), \sum_{l=1}^{K} 1(M^{(4)}(s_l) = j))}{K^2 p_i p_j}$$

$$= \frac{\sum_{k=1}^{K} \sum_{l=1}^{K} \text{Cov}(1(M^{(4)}(s_k) = i), 1(M^{(4)}(s_l) = j))}{K^2 p_i p_j}$$

$$= \frac{-n_i n_j}{K}. \quad (10)$$

In the derivation above, we use

$$\text{Cov}(1(M^{(4)}(s_k) = i), 1(M^{(4)}(s_l) = j)) = 0 \quad \text{when } k \neq l.$$  

Finally, we compute the variance of $\hat{n}_2$ as

$$\text{Var}(\hat{n}_2) = \text{Var}(A_3 - \hat{n}_4 - 2\hat{n}_5 - 4\hat{n}_6) = \text{Var}(\hat{n}_4 + 2\hat{n}_5 + 4\hat{n}_6) + 4\text{Cov}(\hat{n}_4, \hat{n}_5) + 8\text{Cov}(\hat{n}_4, \hat{n}_6) + 16\text{Cov}(\hat{n}_5, \hat{n}_6).$$

Using (9) and (10), then we have

$$\text{Var}(\hat{n}_2) = \frac{1}{K} \left( \frac{n_4}{p_4} + 4\frac{n_5}{p_5} + 16\frac{n_6}{p_6} - (n_4 + 2n_5 + 4n_6)^2 \right).$$

**Proof of Theorem 4**

Let $\phi^{(1)}(s)$ denote the number of ways to sample a 4-node CIS $s$ by MOSS-4Min. Then, we have $\tilde{p}(s) = \phi^{(1)}(s) \times \frac{1}{\sigma^{(u)}} \times \frac{1}{\sigma^{(v)}} \times \frac{1}{\sigma^{(w)}} \times \frac{1}{\sigma^{(t)}} = \phi^{(1)}(s) \Gamma^{-1}$. We compute $\phi^{(1)}(s_1) = 2$, $\phi^{(1)}(s_2) = 2$, and $\phi^{(1)}(s_3) = 6$ for cases $s_1 \in C_4^{(4)}$, $s_2 \in C_5^{(4)}$, and $s_3 \in C_6^{(4)}$, respectively.

**Proof of Theorem 6**

As shown in Fig. 8, we find that there exist two ways to sample a subgraph isomorphic to motif $M_5^{(5)}$ by T-5. Each one happens with probability $\rho^{(3)}(u) \times \sigma^{(u)} \times \frac{1}{\sigma^{(w)}} \times \frac{1}{\sigma^{(t)}} = \frac{1}{17}$. For a 5-node CIS $s$ isomorphic to motif $M_5^{(5)}$, $s$ has $\phi^{(1)}(s_1)$ subgraphs isomorphic to motif $M_5^{(5)}$, $1 \leq i \leq 21$. Therefore, the probability of sampling $s$ is $\frac{2\phi^{(1)}(s_1)}{17}$.  

**Proof of Theorem 7**

For $i \in \Omega_1$ and $1 \leq k \leq K_1$, we have

$$P(M_5^{(5)}(s_k^{(1)}) = i) = \sum_{s \in C_5^{(5)}} P(s_k^{(1)} = s) 1(M_5^{(5)}(s_k^{(1)}) = i) = p_k^{(1)} \eta_i.$$  

Since $s_1^{(1)}, \ldots, s_{K_1}^{(1)}$ are sampled independently, the random variable $m_k^{(1)}$ follows the binomial distribution with parameters $K_1$ and $p_k^{(1)} \eta_i$. Then, the expectation and variance of $m_k^{(1)}$ are

$$E(m_k^{(1)}) = K_1 p_k^{(1)} \eta_i,$$

and

$$\text{Var}(m_k^{(1)}) = K_1 p_k^{(1)} \eta_i (1 - p_k^{(1)} \eta_i). \quad (11)$$

Therefore, the expectation and variance of $\eta_1^{(1)}$ are computed as

$$E(\eta_1^{(1)}) = E \left( \frac{m_1^{(1)}}{K_1 p_1^{(1)}} \right) = \frac{E(m_1^{(1)})}{K_1 p_1^{(1)}} = \eta_i.$$
For $i \in \Omega_2$ and $1 \leq k \leq K_2$, we have

$$P(M^{(5)}(s_k^{(2)}) = i) = \sum_{s \in C_i^{(5)}} P(s^{(2)} = s) \mathbf{1}(M^{(5)}(s_k^{(2)}) = i) = p_i^{(2)} \eta_i.$$  

$s_1^{(2)}, \ldots, s_{K_2}^{(2)}$ are sampled independently, therefore the random variable $m_i^{(2)}$ follows the binomial distribution with parameters $K_2$ and $p_i^{(2)} \eta_i$. Then, the expectation and variance of $m_i^{(2)}$ are

$$E(m_i^{(2)}) = K_2 p_i^{(2)} \eta_i,$$

and

$$Var(m_i^{(2)}) = K_2 p_i^{(2)} (1 - p_i^{(2)} \eta_i).$$

Thus, the expectation and variance of $\eta_i^{(2)}$ are computed as

$$E(\eta_i^{(2)}) = E \left( \frac{m_i^{(2)}}{K_2 p_i^{(2)}} \right) = \frac{E(m_i^{(2)})}{K_2 p_i^{(2)}} = \eta_i,$$

and

$$Var(\eta_i^{(2)}) = Var \left( \frac{m_i^{(2)}}{K_2 p_i^{(2)}} \right) = \frac{Var(m_i^{(2)})}{K_2 p_i^{(2)}}.$$  

For $i \neq j$ and $i, j \in \Omega_2$, the covariance of $\eta_i^{(2)}$ and $\eta_j^{(2)}$ is

$$Cov(\eta_i^{(2)}, \eta_j^{(2)}) = \frac{\eta_i \eta_j}{K_2}.$$

In the derivation above, we use

$$E(1(M^{(5)}(s_k^{(1)}) = i), 1(M^{(5)}(s_l^{(1)}) = j)) = 0, \quad k \neq l,$$

and

$$Cov(1(M^{(5)}(s_k^{(1)}) = i), 1(M^{(5)}(s_l^{(1)}) = j)) = 0 - p_i^{(1)} \eta_i p_j^{(1)} \eta_j = -p_i^{(1)} p_j^{(1)} \eta_i \eta_j.$$

**Proof of Theorem 9**

As shown in Fig. 9, we can see that there exist two ways to sample a subgraph isomorphic to motif $M^{(5)}_k$ by our Path-5 sampling method. Each one happens with probability $\rho_i^{(2)}(s_k) \times \tau_i^{(u)}(s_k) \times \mu_i^{(u,w)}(s_k) \times \frac{1}{d_{a-1}} \times \frac{1}{d_{a-1}} = \frac{1}{\Gamma(5)}$. For a 5-node CIS $s$ isomorphic to the $i$-th 5-node motif, $s$ has $\phi_i^{(2)}$ subgraphs isomorphic to motif $M^{(5)}_k$, $1 \leq i \leq 21$. Thus, the probability of Path-5 sampling $s$ is $\frac{2\phi_i^{(2)}}{\Gamma(5)}$.

**Proof of Theorem 8**

For $i \in \Omega_2$ and $1 \leq k \leq K_2$, we have

$$P(M^{(5)}(s_k^{(2)}) = i) = \sum_{s \in C_i^{(5)}} P(s^{(2)} = s) \mathbf{1}(M^{(5)}(s_k^{(2)}) = i) = p_i^{(2)} \eta_i.$$  

$s_1^{(2)}, \ldots, s_{K_2}^{(2)}$ are sampled independently, therefore the random variable $m_i^{(2)}$ follows the binomial distribution with parameters $K_2$ and $p_i^{(2)} \eta_i$. Then, the expectation and variance of $m_i^{(2)}$ are

$$E(m_i^{(2)}) = K_2 p_i^{(2)} \eta_i,$$

and

$$Var(m_i^{(2)}) = K_2 p_i^{(2)} (1 - p_i^{(2)} \eta_i).$$

Thus, the expectation and variance of $\eta_i^{(2)}$ are computed as

$$E(\eta_i^{(2)}) = E \left( \frac{m_i^{(2)}}{K_2 p_i^{(2)}} \right) = \frac{E(m_i^{(2)})}{K_2 p_i^{(2)}} = \eta_i,$$

and

$$Var(\eta_i^{(2)}) = Var \left( \frac{m_i^{(2)}}{K_2 p_i^{(2)}} \right) = \frac{Var(m_i^{(2)})}{K_2 p_i^{(2)}}.$$  

For $i \neq j$ and $i, j \in \Omega_2$, the covariance of $\eta_i^{(2)}$ and $\eta_j^{(2)}$ is

$$Cov(\eta_i^{(2)}, \eta_j^{(2)}) = \frac{\eta_i \eta_j}{K_2}.$$

In the derivation above, we use

$$E(1(M^{(5)}(s_k^{(1)}) = i), 1(M^{(5)}(s_l^{(1)}) = j)) = 0, \quad k \neq l,$$

and

$$Cov(1(M^{(5)}(s_k^{(1)}) = i), 1(M^{(5)}(s_l^{(1)}) = j)) = 0 - p_i^{(1)} \eta_i p_j^{(1)} \eta_j = -p_i^{(1)} p_j^{(1)} \eta_i \eta_j.$$  

**Proof of Theorem 10**

For $i \in \Omega_1 \cup \Omega_2$, Theorems 7 and 8 tell us that $\eta_i^{(1)}$ and $\eta_i^{(2)}$ are unbiased estimators of $\eta_i^{(1)}$, and they are independent. Moreover, $\lambda_i^{(1)} + \lambda_i^{(2)} = 1$. Therefore, we easily find that $\eta_i$ is also an unbiased estimator of $\eta_i^{(1)}$, and its variance is $\eta_i^{(1)}$. Next, we study the expectation and variance of $\eta_2$. The expectation of $\eta_2$ is

$$E(\eta_2) = \Lambda_4 - \sum_{i \in \Omega_2} \phi_i^{(3)} E(\eta_i) = \Lambda_4 - \sum_{i \in \Omega_2} \phi_i^{(3)} \eta_i = \eta_2.$$
Next, we compute the covariance of $\hat{\eta}_i$ and $\hat{\eta}_j$ for $i, j \in \Omega_1 \cup \Omega_2$ and $i \neq j$. For any $i, j \in \Omega_1 \cup \Omega_2$, we have $\text{Cov}(\hat{\eta}_i^{(1)}, \hat{\eta}_j^{(2)}) = 0$ because $\hat{\eta}_i^{(1)}$ and $\hat{\eta}_j^{(2)}$ are independent. Thus, we have $\text{Cov}(\hat{\eta}_i, \hat{\eta}_j) = \text{Cov}(\hat{\eta}_i^{(1)}, \hat{\eta}_j^{(2)}) = 0$ when $i \in \Omega_1 - \Omega_2$ and $j \in \Omega_2 - \Omega_1$. When $i \in \Omega_1 - \Omega_2$ and $j \in \Omega_1 \cap \Omega_2$, we have

$$\text{Cov}(\hat{\eta}_i, \hat{\eta}_j) = \text{Cov}(\hat{\eta}_i^{(1)}, \lambda_j^{(1)} \hat{\eta}_j^{(1)} + \lambda_j^{(2)} \hat{\eta}_j^{(2)}) = \lambda_j^{(1)} \text{Cov}(\hat{\eta}_i^{(1)}, \hat{\eta}_j^{(1)}) + \lambda_j^{(2)} \text{Cov}(\hat{\eta}_i^{(1)}, \hat{\eta}_j^{(2)}) = -\eta_i \eta_j \lambda_j^{(1)} \left(\frac{\lambda_j^{(1)}}{K_1} + \frac{\lambda_j^{(2)}}{K_2}\right).$$

Similarly, we have $\text{Cov}(\hat{\eta}_i, \hat{\eta}_j) = -\frac{\lambda^{(2)} \eta_i \eta_j}{K_2}$ when $i \in \Omega_1 \cap \Omega_2$ and $j \in \Omega_2 - \Omega_1$. When $i, j \in \Omega_1 \cap \Omega_2$ and $i \neq j$, we have

$$\text{Cov}(\hat{\eta}_i, \hat{\eta}_j) = \text{Cov}(\lambda_i^{(1)} \hat{\eta}_i^{(1)} + \lambda_i^{(2)} \hat{\eta}_i^{(2)}, \lambda_j^{(1)} \hat{\eta}_j^{(1)} + \lambda_j^{(2)} \hat{\eta}_j^{(2)}) = \lambda_i^{(1)} \lambda_j^{(1)} \text{Cov}(\hat{\eta}_i^{(1)}, \hat{\eta}_j^{(1)}) + \lambda_i^{(2)} \lambda_j^{(2)} \text{Cov}(\hat{\eta}_i^{(2)}, \hat{\eta}_j^{(2)}) = -\eta_i \eta_j \lambda_i^{(1)} \left(\frac{\lambda_i^{(1)}}{K_1} + \frac{\lambda_i^{(2)}}{K_2}\right).$$

Finally, the variance of $\hat{\eta}_2$ is computed as

$$\text{Var}(\hat{\eta}_2) = \text{Var}(\lambda_4 - \sum_{i \in \Omega_3} \phi_i^{(3)} \hat{\eta}_i) = \sum_{i \in \Omega_3} \text{Var}(\phi_i^{(3)} \hat{\eta}_i) + \sum_{i \in \Omega_3} \sum_{j \neq i, j \in \Omega_3} \text{Cov}(\phi_i^{(3)} \hat{\eta}_i, \phi_j^{(3)} \hat{\eta}_j) = \sum_{i \in \Omega_3} (\phi_i^{(3)})^2 \text{Var}(\hat{\eta}_i) + \sum_{i \in \Omega_3} \sum_{j \neq i, j \in \Omega_3} \phi_i^{(3)} \phi_j^{(3)} \text{Cov}(\hat{\eta}_i, \hat{\eta}_j).$$

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