Hypergraph Motifs: Concepts, Algorithms, and Discoveries

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ABSTRACT

Hypergraphs naturally represent group interactions, which are omnipresent in many domains: collaborations of researchers, co-purchases of items, joint interactions of proteins, to name a few. In this work, we propose tools for answering the following questions in a systematic manner: (Q1) what are structural design principles of real-world hypergraphs? (Q2) how can we compare local structures of hypergraphs of different sizes? (Q3) how can we identify domains which hypergraphs are from? We first define hy*pergraph motifs* (h-motifs), which describe the connectivity patterns of three connected hyperedges. Then, we define the significance of each h-motif in a hypergraph as its occurrences relative to those in properly randomized hypergraphs. Lastly, we define the *characteristic profile* (CP) as the vector of the normalized significance of every h-motif. Regarding Q1, we find that h-motifs' occurrences in 11 real-world hypergraphs from 5 domains are clearly distinguished from those of randomized hypergraphs. In addition, we demonstrate that CPs capture local structural patterns unique to each domain, and thus comparing CPs of hypergraphs addresses Q2 and Q3. Our algorithmic contribution is to propose MoCHy, a family of parallel algorithms for counting h-motifs' occurrences in a hypergraph. We theoretically analyze their speed and accuracy, and we show empirically that the advanced approximate version MoCHy-A⁺ is up to $25 \times$ more accurate and $32 \times$ faster than the basic approximate and exact versions, respectively.

PVLDB Reference Format:

Geon Lee, Jihoon Ko, and Kijung Shin. Hypergraph Motifs: Concepts, Algorithms, and Discoveries. *PVLDB*, 13(11): 2256-2269, 2020.

DOI: https://doi.org/10.14778/3407790.3407823

1. INTRODUCTION

Complex systems consisting of pairwise interactions between individuals or objects are naturally expressed in the form of graphs. Nodes and edges, which compose a graph, represent individuals (or objects) and their pairwise interactions, respectively. Thanks to their powerful expressiveness,

Proceedings of the VLDB Endowment, Vol. 13, No. 11 ISSN 2150-8097.

DOI: https://doi.org/10.14778/3407790.3407823

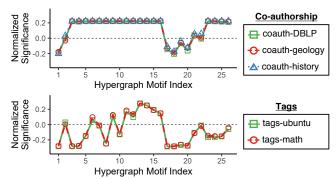


Figure 1: Distributions of h-motifs' instances precisely characterize local structural patterns of real-world hypergraphs. Note that the hypergraphs from the same domains have similar distributions, while the hypergraphs from different domains do not. See Section 4.3 for details.

graphs have been used in a wide variety of fields, including social network analysis, web, bioinformatics, and epidemiology. Global structural patterns of real-world graphs, such as power-law degree distribution [10, 24] and six degrees of separation [33, 66], have been extensively investigated.

In addition to global patterns, real-world graphs exhibit patterns in their local structures, which differentiate graphs in the same domain from random graphs or those in other domains. Local structures are revealed by counting the occurrences of different network motifs [45, 46], which describe the patterns of pairwise interactions between a fixed number of connected nodes (typically 3, 4, or 5 nodes). As a fundamental building block, network motifs have played a key role in many analytical and predictive tasks, including community detection [13, 43, 62, 68], classification [20, 39, 45], and anomaly detection [11, 57].

Despite the prevalence of graphs, interactions in many complex systems are groupwise rather than pairwise: collaborations of researchers, co-purchases of items, joint interactions of proteins, tags attached to the same web post, to name a few. These group interactions cannot be represented by edges in a graph. Suppose three or more researchers coauthor a publication. This co-authorship cannot be represented as a single edge, and creating edges between all pairs of the researchers cannot be distinguished from multiple papers coauthored by subsets of the researchers.

This inherent limitation of graphs is addressed by hypergraphs, which consist of nodes and hyperedges. Each hyperedge is a subset of any number of nodes, and it represents a group interaction among the nodes. For example, the coauthorship relations in Figure 2(a) are naturally represented as

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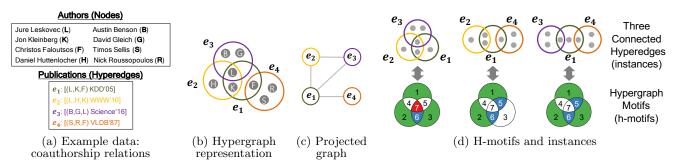


Figure 2: (a) Example: co-authorship relations. (b) Hypergraph: the hypergraph representation of (a). (c) Projected Graph: the projected graph of (b). (d) Hypergraph Motifs: example h-motifs and their instances in (b).

Table 1: Frequently-used symbols.

Notation	Definition
$G = (V, E)$ $E = \{e_1, \dots, e_{ E }\}$ E_v	hypergraph with nodes V and hyperedges E set of hyperedges set of hyperedges that contains a node v
$\wedge \\ \wedge_{ij}$	set of hyperwedges in G hyperwedge consisting of e_i and e_j
$ \bar{G} = (E, \wedge, \omega) \\ \omega(\wedge_{ij}) \\ N_{e_i} $	projected graph of G the number of nodes shared between e_i and e_j set of neighbors of e_i in \overline{G}
$\frac{h(\{e_i, e_j, e_k\})}{M[t]}$	h-motif corresponding to an instance $\{e_i, e_j, e_k\}$ count of h-motif t's instances

the hypergraph in Figure 2(b). In the hypergraph, seminar work [40] coauthored by Jure Leskovec (L), Jon Kleinberg (K), and Christos Faloutsos (F) is expressed as the hyperedge $e_1 = \{L, K, F\}$, and it is distinguished from three papers coauthored by each pair, which, if they exist, can be represented as three hyperedges $\{K, L\}, \{F, L\}, \text{ and } \{F, K\}$.

The successful investigation and discovery of local structural patterns in real-world graphs motivate us to explore local structural patterns in real-world hypergraphs. However, network motifs, which proved to be useful for graphs, are not trivially extended to hypergraphs. Due to the flexibility in the size of hyperedges, there can be infinitely many patterns of interactions among a fixed number of nodes, and other nodes can also be associated with these interactions.

In this work, taking these challenges into consideration, we define 26 hypergraph motifs (h-motifs) so that they describe connectivity patterns of three connected hyperedges (rather than nodes). As seen in Figure 2(d), h-motifs describe the connectivity pattern of hyperedges e_1 , e_2 , and e_3 by the emptiness of seven subsets: $e_1 \setminus e_2 \setminus e_3$, $e_2 \setminus e_3 \setminus e_1$, $e_3 \setminus e_1 \setminus e_2$, $e_1 \cap e_2 \setminus e_3$, $e_2 \cap e_3 \setminus e_1$, $e_3 \cap e_1 \setminus e_2$, and $e_1 \cap e_2 \cap e_3$. As a result, every connectivity pattern is described by a unique h-motif, independently of the sizes of hyperedges. While this work focuses on connectivity patterns of three hyperedges, h-motifs are easily extended to four or more hyperedges.

We count the number of each h-motif's instances in 11 real-world hypergraphs from 5 different domains. Then, we measure the significance of each h-motif in each hypergraph by comparing the count of its instances in the hypergraph against the counts in properly randomized hypergraphs. Lastly, we compute the *characteristic profile* (CP) of each hypergraph, defined as the vector of the normalized significance of every h-motif. Comparing the counts and CPs of different hypergraphs leads to the following observations:

- Structural design principles of real-world hypergraphs that are captured by frequencies of different h-motifs are clearly distinguished from those of randomized hypergraphs.
- Hypergraphs from the same domains have similar CPs,

while hypergraphs from different domains have distinct CPs (see Figure 1). In other words, CPs successfully capture local structure patterns unique to each domain.

Our algorithmic contribution is to design MoCHy (Motif Counting in Hypergraphs), a family of parallel algorithms for counting h-motifs' instances, which is the computational bottleneck of the aforementioned process. Note that since non-pairwise interactions are taken into consideration, counting the instances of h-motifs is more challenging than counting the instances of network motifs, which are defined solely based on pairwise interactions. We provide one exact version, named MoCHy-E, and two approximate versions, named MoCHy-A and MoCHy-A⁺. Empirically, MoCHy-A⁺ is up to $25 \times$ more accurate than MoCHy-A, and it is up to $32 \times$ faster than MoCHy-E, with little sacrifice of accuracy. These empirical results are consistent with our theoretical analyses.

In summary, our contributions are summarized as follow:

- Novel Concepts: We propose h-motifs, the counts of whose instances capture local structures of hypergraphs, independently of the sizes of hyperedges or hypergraphs.
- Fast and Provable Algorithms: We develop MoCHy, a family of parallel algorithms for counting h-motifs' instances. We show theoretically and empirically that the advanced version significantly outperforms the basic ones, providing a better trade-off between speed and accuracy.
- **Discoveries in** 11 **Real-world Hypergraphs:** We show that h-motifs and CPs reveal local structural patterns that are shared by hypergraphs from the same domains but distinguished from those of random hypergraphs and hypergraphs from other domains (see Figure 1).

Reproducibility: The code and datasets used in this work are available at https://github.com/geonlee0325/MoCHy.

In Section 2, we introduce h-motifs and characteristic profiles. In Section 3, we present exact and approximate algorithms for counting instances of h-motifs, and we analyze their theoretical properties. In Section 4, we provide experimental results. After discussing related work in Section 5, we offer conclusions in Section 6.

2. PROPOSED CONCEPTS

In this section, we introduce the proposed concepts: hypergraph motifs and characteristic profiles. Refer Table 1 for the notations frequently used throughout the paper.

2.1 Preliminaries and Notations

We define some preliminary concepts and their notations. **<u>Hypergraph</u>** Consider a hypergraph G = (V, E), where Vand $E := \{e_1, e_2, ..., e_{|E|}\}$ are sets of nodes and hyperedges, respectively. Each hyperedge $e_i \in E$ is a non-empty subset

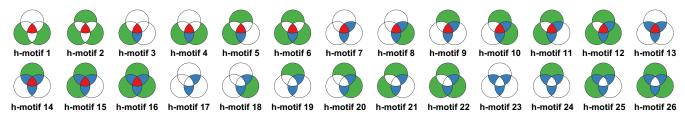


Figure 3: The 26 h-motifs studied in this work. Note that h-motifs 17 - 22 are open, while the others are closed.



Figure 4: The h-motifs whose instances contain duplicated hyperedges.

of V, and we use $|e_i|$ to denote the number of nodes in it. For each node $v \in V$, we use $E_v := \{e_i \in E : v \in e_i\}$ to denote the set of hyperedges that include v. We say two hyperedges e_i and e_j are *adjacent* if they share any member, i.e., if $e_i \cap e_j \neq \emptyset$. Then, for each hyperedge e_i , we denote the set of hyperedges adjacent to e_i by $N_{e_i} := \{e_j \in E : e_i \cap e_j \neq \emptyset\}$ and the number of such hyperedges by $|N_{e_i}|$. Similarly, we say three hyperedges e_i , e_j , and e_k are *connected* if one of them is adjacent to two the others.

Hyperwedges: We define a hyperwedge as an unordered pair of adjacent hyperedges. We denote the set of hyperwedges in G by $\wedge := \{\{e_i, e_j\} \in {E \choose 2} : e_i \cap e_j \neq \emptyset\}$. We use $\wedge_{ij} \in \wedge$ to denote the hyperwedge consisting of e_i and e_j . In the example hypergraph in Figure 2(b), there are four hyperwedges: \wedge_{12} , \wedge_{13} , \wedge_{23} , and \wedge_{14} .

Projected Graph: We define the projected graph of G = (V, E) as $\overline{G} = (E, \wedge, \omega)$ where \wedge is the set of hyperwedges and $\omega(\wedge_{ij}) := |e_i \cap e_j|$. That is, in the projected graph \overline{G} , hyperedges in G act as nodes, and two of them are adjacent if and only if they share any member. Note that for each hyperedge $e_i \in E$, N_{e_i} is the set of neighbors of e_i in \overline{G} , and $|N_{e_i}|$ is its degree in \overline{G} . Figure 2(c) shows the projected graph of the example hypergraph in Figure 2(b).

2.2 Hypergraph Motifs

We introduce hypergraph motifs, which are basic building blocks of hypergraphs, with related concepts. Then, we discuss their properties and generalization.

Definition and Representation: Hypergraph motifs (or h-motifs in short) are for describing the connectivity patterns of three connected hyperedges. Specifically, given a set $\{e_i, e_j, e_k\}$ of three connected hyperedges, h-motifs describe its connectivity pattern by the emptiness of the following seven sets: (1) $e_i \setminus e_j \setminus e_k$, (2) $e_j \setminus e_k \setminus e_i$, (3) $e_k \setminus e_i \setminus e_j$, (4) $e_i \cap e_j \setminus e_k$, (5) $e_j \cap e_k \setminus e_i$, (6) $e_k \cap e_i \setminus e_j$, and (7) $e_i \cap e_j \cap e_k$. Formally, a h-motif is defined as a binary vector of size 7 whose elements represent the emptiness of the above sets, respectively, and as seen in Figure 2(d), h-motifs are naturally represented in the Venn diagram. While there can be 2^7 h-motifs, 26 h-motifs remain once we exclude symmetric ones, those with duplicated hyperedges (see Figure 4), and those cannot be obtained from connected hyperedges. The 26 cases, which we call *h*-motif 1 through *h*-motif 26, are visualized in the Venn diagram in Figure 3.

Instances, Open h-motifs, and Closed h-motifs: Consider a hypergraph G = (V, E). A set of three connected hyperedges is an *instance* of h-motif t if their connectivity pattern corresponds to h-motif t. The count of each h-motif's instances is used to characterize the local structure of G,

as discussed in the following sections. A h-motif is *closed* if all three hyperedges in its instances are adjacent to (i.e., overlapped with) each other. If its instances contain two non-adjacent (i.e., disjoint) hyperedges, a h-motif is *open*. In Figure 3, h-motifs 17 - 22 are open; the others are closed. **Properties of h-motifs:** From the definition of h-motifs, the following desirable properties are immediate:

- Exhaustive: h-motifs capture connectivity patterns of *all possible* three connected hyperedges.
- Unique: connectivity pattern of any three connected hyperedges is captured by *at most one* h-motif.
- **Size Independent:** h-motifs capture connectivity patterns *independently of the sizes of hyperedges*. Note that there can be infinitely many combinations of sizes of three connected hyperedges.

Note that the exhaustiveness and the uniqueness imply that connectivity pattern of any three connected hyperedges is captured by *exactly one* h-motif.

Why Non-pairwise Relations?: Non-pairwise relations (e.g., the emptiness of $e_1 \cap e_2 \cap e_3$ and $e_1 \setminus e_2 \setminus e_3$) play a key role in capturing the local structural patterns of real-world hypergraphs. Taking only the pairwise relations (e.g., the emptiness of $e_1 \cap e_2$, $e_1 \setminus e_2$, and $e_2 \setminus e_1$) into account limits the number of possible connectivity patterns of three distinct hyperedges to just eight,¹ significantly limiting their expressiveness and thus usefulness. Specifically, 12 (out of 26) h-motifs have the same pairwise relations, while their occurrences and significances vary substantially in real-world hypergraphs. For example, in Figure 2, $\{e_1, e_2, e_4\}$ and $\{e_1, e_3, e_4\}$ have the same pairwise relations, while their connectivity patterns are distinguished by h-motifs.

Generalization to More than 3 Hyperedges: The concept of h-motifs is easily generalized to four or more hyperedges. For example, a h-motif for four hyperedges can be defined as a binary vector of size 15 indicating the emptiness of each region in the Venn diagram for four sets. After excluding disconnected ones, symmetric ones, and those with duplicated hyperedges, there remain 1,853 and 18,656,322 h-motifs for four and five hyperedges, respectively, as discussed in detail in Appendix F of [1]. This work focuses on the h-motifs for three hyperedges, which are already capable of characterizing local structures of real-world hypergraphs, as shown empirically in Section 4.

2.3 Characteristic Profile (CP)

What are the structural design principles of real-world hypergraphs distinguished from those of random hypergraphs? Below, we introduce the characteristic profile (CP), which is a tool for answering the above question using h-motifs.

Randomized Hypergraphs: While one might try to characterize the local structure of a hypergraph by absolute <u>counts of each h-motif's</u> instances in it, some h-motifs may ¹Note that using the conventional network motifs in projected graphs limits this number to two.

naturally have many instances. Thus, for more accurate characterization, we need random hypergraphs to be compared against real-world hypergraphs. We obtain such random hypergraphs by randomizing the compared real-world hypergraph. To this end, we represent the hypergraph G =(V, E) as the bipartite graph G' where V and E are the two subsets of nodes, and there exists an edge between $v \in V$ and $e \in E$ if and only if $v \in e$ That is, G' = (V', E') where $V' := V \cup E$ and $E' := \{(v, e) \in V \times E : v \in e\}$. Then, we use the Chung-Lu model to generate bipartite graphs where the degree distribution of G' is well preserved [6]. Reversely, from each of the generated bipartite graphs, we can obtain a randomized hypergraph where the degree (i.e., the number of hyperedges that each node belongs to) distribution of nodes and the size distribution of hyperedges in G are well preserved. We provide the pseudocode and the distributions in the randomized hypergraphs in Appendix D of [1].

Significance of H-motifs: We measure the significance of each h-motif in a hypergraph by comparing the count of its instances against the count of them in randomized hypergraphs. Specifically, the *significance* of a h-motif t in a hypergraph G is defined as

$$\Delta_t := \frac{M[t] - M_{rand}[t]}{M[t] + M_{rand}[t] + \epsilon},\tag{1}$$

where M[t] is the number of instances of h-motif t in G, and $M_{rand}[t]$ is the average number of instances of h-motif t in randomized hypergraphs. We fixed ϵ to 1 throughout this paper. This way of measuring significance was proposed for network motifs as an alternative of normalized Z scores, which heavily depend on the graph size [45].

Characteristic Profile (CP): By normalizing and concatenating the significances of all h-motifs in a hypergraph, we obtain the characteristic profile (CP), which summarizes the local structural pattern of the hypergraph. Specifically, the *characteristic profile* of a hypergraph G is a vector of size 26, where each t-th element is

$$CP_t := \frac{\Delta_t}{\sqrt{\sum_{t=1}^{26} \Delta_t^2}}.$$
(2)

Note that, for each t, CP_t is between -1 and 1. The CP is used in Section 4.3 to compare the local structural patterns of real-world hypergraphs from diverse domains.

3. PROPOSED ALGORITHMS

Given a hypergraph, how can we count the instances of each h-motif? Once we count them in the original and randomized hypergraphs, the significance of each h-motif and the CP are obtained immediately by Eq. (1) and Eq. (2).

In this section, we present MoCHy (Motif Counting in Hypergraphs), which is a family of parallel algorithms for counting the instances of each h-motif in the input hypergraph. We first describe hypergraph projection, which is a preprocessing step of every version of MoCHy. Then, we present MoCHy-E, which is for exact counting. After that, we present two different versions of MoCHy-A, which are sampling-based algorithms for approximate counting. Lastly, we discuss parallel and on-the-fly implementations.

Throughout this section, we use $h(\{e_i, e_j, e_k\})$ to denote the h-motif that describes the connectivity pattern of an hmotif instance $\{e_i, e_j, e_k\}$. We also use M[t] to denote the count of instances of h-motif t.

Algorithm 1: Hypergraph Projection (Preprocess)

 $\begin{array}{c|c} \textbf{Input} & : \text{input hypergraph: } G = (V, E) \\ \textbf{Output: projected graph: } \bar{G} = (E, \wedge, \omega) \\ \textbf{1} & \wedge \leftarrow \varnothing \\ \textbf{2} & \omega \leftarrow \text{map whose default value is 0} \\ \textbf{3} & \textbf{for each hyperedge } e_i \in E \quad \textbf{do} \\ \textbf{4} & \quad \textbf{for each node } v \in e_i \quad \textbf{do} \\ \textbf{5} & \quad | \quad \textbf{for each hyperedge } e_j \in E_v \text{ where } j > i \quad \textbf{do} \\ \textbf{6} & \quad | \quad \wedge \leftarrow \wedge \cup \{\wedge_{ij}\} \\ \textbf{7} & \quad | \quad | \quad \omega(\wedge_{ij}) = \omega(\wedge_{ij}) + 1 \\ \textbf{8} \text{ return } \bar{G} = (E, \wedge, \omega) \end{array}$

Remarks: The problem of counting h-motifs' occurrences bears some similarity to the classic problem of counting network motifs' occurrences. However, different from network motifs, which are defined solely based on pairwise interactions, h-motifs are defined based on triple-wise interactions, h-motifs are defined based on triple-wise interactions (e.g., $e_i \cap e_j \cap e_k$). One might hypothesize that our problem can easily be reduced to the problem of counting the occurrences of network motifs, and thus existing solutions (e.g., [18, 50]) are applicable to our problem. In order to examine this possibility, we consider the following two attempts:

- (a) Represent pairwise relations between hyperedges using the projected graph, where each edge $\{e_i, e_j\}$ indicates $e_i \cap e_j \neq \emptyset$.
- (b) Represent pairwise relations between hyperedges using the directed projected graph where each directed edge $e_i \rightarrow e_j$ indicates $e_i \cap e_j \neq \emptyset$ and at the same time $e_i \not\subset e_j$.

The number of possible connectivity patterns (i.e., network motifs) among three distinct connected hyperedges is just two (i.e., closed and open triangles) and eight in (a) and (b), respectively. In both cases, instances of multiple h-motifs are not distinguished by network motifs, and the occurrences of h-motifs can not be inferred from those of network motifs.

In addition, another computational challenge stems from the fact that triple-wise and even pair-wise relations between hyperedges need to be computed from the input hypergraph, while pairwise relations between edges are given in graphs. This challenge necessitates the precomputation of partial relations, described in the next subsection.

3.1 Hypergraph Projection (Algorithm 1)

As a preprocessing step, every version of MoCHy builds the projected graph $\overline{G} = (E, \wedge, \omega)$ (see Section 2.1) of the input hypergraph G = (V, E), as described in Algorithm 1. To find the neighbors of each hyperedge e_i (line 3), the algorithm visits each hyperedge e_j that contains v and satisfies j > i (line 5) for each node $v \in e_i$ (line 4). Then for each such e_j , it adds $\wedge_{ij} = \{e_i, e_j\}$ to \wedge and increments $\omega(\wedge_{ij})$ (lines 6 and 7). The time complexity of this preprocessing step is given in Lemma 1.

Lemma 1 (Complexity of Hypergraph Projection). The time complexity of Algorithm 1 is $O(\sum_{\Lambda_{ij} \in \Lambda} |e_i \cap e_j|)$.

Proof. If all sets and maps are implemented using hash tables, lines 6 and 7 take O(1) time, and they are executed $|e_i \cap e_j|$ times for each $\wedge_{ij} \in \wedge$.

Since $|\wedge| < \sum_{e_i \in E} |N_{e_i}|$ and $|e_i \cap e_j| \le |e_i|$, Eq. (3) holds.

$$\sum_{\bigwedge_{ij\in\bigwedge}} |e_i \cap e_j| < \sum_{e_i\in E} (|e_i| \cdot |N_{e_i}|).$$
(3)

Algorithm 2: MoCHy-E: Exact H-motif Counting

3.2 Exact H-motif Counting (Algorithm 2)

We present MoCHy-E (MoCHy Exact), which counts the instances of each h-motif exactly. The procedures of MoCHy-E are described in Algorithm 2. For each hyperedge $e_i \in E$ (line 2), each unordered pair $\{e_j, e_k\}$ of its neighbors, where $\{e_i, e_j, e_k\}$ is an h-motif instance, is considered (line 3). If $e_j \cap e_k = \emptyset$ (i.e., if the corresponding h-motif is open), $\{e_i, e_j, e_k\}$ is considered only once. However, if $e_j \cap e_k \neq \emptyset$ (i.e., if the corresponding h-motif is closed), $\{e_i, e_j, e_k\}$ is considered two more times (i.e., when e_j is chosen in line 2 and when e_k is chosen in line 2). Based on these observations, given an h-motif instance $\{e_i, e_j, e_k\}$, the corresponding $M[h(\{e_i, e_j, e_k\})]$ is incremented (line 5) only if $e_j \cap e_k = \emptyset$ or $i < \min(j, k)$ (line 4). This guarantees that each instance is counted exactly once. The time complexity of MoCHy-E is given in Theorem 1, which uses Lemma 2.

Lemma 2 (Time Complexity of Computing $h(\{e_i, e_j, e_k\})$). Given the input hypergraph G = (V, E) and its projected graph $\overline{G} = (E, \wedge, \omega)$, for each h-motif instance $\{e_i, e_j, e_k\}$, computing $h(\{e_i, e_j, e_k\})$ takes $O(\min(|e_i|, |e_j|, |e_k|))$ time.

Proof. Assume $|e_i| = \min(|e_i|, |e_j|, |e_k|)$, without loss of generality, and all sets and maps are implemented using hash tables. As defined in Section 2.2, $h(\{e_i, e_j, e_k\})$ is computed in O(1) time from the emptiness of the following sets: (1) $e_i \setminus e_j \setminus e_k$, (2) $e_j \setminus e_k \setminus e_i$, (3) $e_k \setminus e_i \setminus e_j$, (4) $e_i \cap e_j \setminus e_k$, (5) $e_j \cap e_k \setminus e_i$, (6) $e_k \cap e_i \setminus e_j$, and (7) $e_i \cap e_j \cap e_k$. We check their emptiness from their cardinalities. We obtain e_i, e_j , and e_k , which are stored in G, and their cardinalities in O(1) time. Similarly, we obtain $|e_i \cap e_j|, |e_j \cap e_k|$, and $|e_k \cap e_i|$, which are stored in \overline{G} , in O(1) time. Then, we compute $|e_i \cap e_j \cap e_k|$ in $O(|e_i|)$ time by checking for each node in e_i whether it is also in both e_j and e_k . From these cardinalities, we obtain the cardinalities of the six other sets in O(1) time as follows:

 $\begin{array}{l} (1) \ |e_i \setminus e_j \setminus e_k| = |e_i| - |e_i \cap e_j| - |e_k \cap e_i| + |e_i \cap e_j \cap e_k|, \\ (2) \ |e_j \setminus e_k \setminus e_i| = |e_j| - |e_i \cap e_j| - |e_j \cap e_k| + |e_i \cap e_j \cap e_k|, \\ (3) \ |e_k \setminus e_i \setminus e_j| = |e_k| - |e_k \cap e_i| - |e_j \cap e_k| + |e_i \cap e_j \cap e_k|, \\ (4) \ |e_i \cap e_j \setminus e_k| = |e_i \cap e_j| - |e_i \cap e_j \cap e_k|, \\ (5) \ |e_j \cap e_k \setminus e_i| = |e_j \cap e_k| - |e_i \cap e_j \cap e_k|, \\ (6) \ |e_k \cap e_i \setminus e_j| = |e_k \cap e_i| - |e_i \cap e_j \cap e_k|. \end{array}$

Hence, the time complexity of computing $h(\{e_i, e_j, e_k\})$ is $O(|e_i|) = O(\min(|e_i|, |e_j|, |e_k|)).$

Theorem 1 (Complexity of MoCHy-E). The time complexity of Algorithm 2 is $O(\sum_{e_i \in E} (|N_{e_i}|^2 \cdot |e_i|)).$

Proof. Assume all sets and maps are implemented using hash tables. The total number of triples $\{e_i, e_j, e_k\}$ considered in line 3 is $O(\sum_{e_i \in E} |N_{e_i}|^2)$. By Lemma 2, for such a triple $\{e_i, e_j, e_k\}$, computing $h(\{e_i, e_j, e_k\})$ takes $O(|e_i|)$

Algorithm 3: MoCHy-E_{ENUM} for H-motif Enumeration

Input : (1) input hypergraph: G = (V, E)(2) projected graph: $\overline{G} = (E, \wedge, \omega)$

Output: h-motif instances and their corresponding h-motifs 1 for each hyperedge $e_i \in E$ do

2 for each unordered hyperedge pair $\{e_j, e_k\} \in \binom{N_{e_i}}{2}$ do

3 **if** $e_j \cap e_k = \emptyset$ or $i < \min(j, k)$ then

4 write $(e_i, e_j, e_k, h(\{e_i, e_j, e_k\}))$

Algorithm 4: MoCHy-A: Approximate H-motif Counting Based on Hyperedge Sampling

(2) projected graph: $\bar{G} = (E, \wedge, \omega)$ (3) number of samples: s Output: estimated count of each h-motif t 's instances: $\bar{M}[t]$ 1 $\bar{M}[t] \leftarrow$ map whose default value is 0 2 for $n \leftarrow 1s$ do 3 $e_i \leftarrow$ sample a uniformly random hyperedge 4 for each hyperedge $e_j \in N_{e_i}$ do 5 $for each hyperedge e_k \in (N_{e_i} \cup N_{e_j} \setminus \{e_i, e_j\}) do$
Output: estimated count of each h-motif t's instances: $\overline{M}[t]$ 1 $\overline{M}[t] \leftarrow$ map whose default value is 0 2 for $n \leftarrow 1s$ do 3 $e_i \leftarrow$ sample a uniformly random hyperedge 4 for each hyperedge $e_j \in N_{e_i}$ do 5 for each hyperedge $e_k \in (N_{e_i} \cup N_{e_i} \setminus \{e_i, e_i\})$ do
1 $\overline{M}[t] \leftarrow$ map whose default value is 0 2 for $n \leftarrow 1s$ do 3 $e_i \leftarrow$ sample a uniformly random hyperedge 4 for each hyperedge $e_j \in N_{e_i}$ do 5 for each hyperedge $e_k \in (N_{e_i} \cup N_{e_i} \setminus \{e_i, e_i\})$ do
2 for $n \leftarrow 1s$ do 3 $e_i \leftarrow \text{sample a uniformly random hyperedge}$ 4 for each hyperedge $e_j \in N_{e_i}$ do 5 for each hyperedge $e_k \in (N_{e_i} \cup N_{e_i} \setminus \{e_i, e_i\})$ do
$\begin{array}{c c} \mathbf{s} & e_i \leftarrow \text{sample a uniformly random hyperedge} \\ \mathbf{for \ each \ hyperedge \ } e_j \in N_{e_i} \ \mathbf{do} \\ \mathbf{for \ each \ hyperedge \ } e_i \in (N_{e_i} \cup N_{e_i} \setminus \{e_i, e_i\}) \ \mathbf{do} \end{array}$
4 for each hyperedge $e_j \in N_{e_i}$ do 5 for each hyperedge $e_k \in (N_{e_i} \cup N_{e_i} \setminus \{e_i, e_j\})$ do
5 for each hyperedge $e_k \in (N_e \cup N_e \setminus \{e_i, e_i\})$ do
5 for each hyperedge $e_k \in (N_{e_i} \cup N_{e_j} \setminus \{e_i, e_j\})$ do
6 if $e_k \notin N_{e_i}$ or $j < k$ then
$\begin{array}{c c c c c c } \mathbf{\hat{s}}_{k} \notin N_{e_{i}} & or j < k \text{ then} \\ \mathbf{\hat{r}}_{k} \notin N_{e_{i}} & or j < k \text{ then} \\ & & & & & & \\ & & & & & & \\ & & & & $
s for each h-motif t do
$\mathbf{g} \mid \bar{M}[t] \leftarrow \bar{M}[t] \cdot rac{ E }{3s}$
10 return M

time. Thus, the total time complexity of Algorithm 2 is $O(\sum_{e_i \in E} (|e_i| \cdot |N_{e_i}|^2))$, which dominates that of the preprocessing step (see Lemma 1 and Eq. (3)).

Extension of MoCHy-E to H-motif Enumeration:

Since MoCHy-E visits all h-motif instances to count them, it is extended to the problem of enumerating every h-motif instance (with its corresponding h-motif), as described in Algorithm 3. The time complexity remains the same.

3.3 Approximate H-motif Counting

We present two different versions of MoCHy-A (MoCHy Approximate), which approximately count the instances of each h-motif. Both versions yield unbiased estimates of the counts by exploring the input hypergraph partially through hyperedge and hyperwedge sampling, respectively.

MoCHy-A: Hyperedge Sampling (Algorithm 4):

MoCHy-A (Algorithm 4) is based on hyperedge sampling. It repeatedly samples s hyperedges from the hyperedge set Euniformly at random with replacement (line 3). For each sampled hyperedge e_i , the algorithm searches for all h-motif instances that contain e_i (lines 4-7), and to this end, the 1-hop and 2-hop neighbors of e_i in the projected graph \bar{G} are explored. After that, for each such instance $\{e_i, e_j, e_k\}$ of h-motif t, the corresponding count $\bar{M}[t]$ is incremented (line 7). Lastly, each estimate $\bar{M}[t]$ is rescaled by multiplying it with $\frac{|E|}{3s}$ (lines 8-9), which is the reciprocal of the expected number of times that each of the h-motif t's instances is counted.² This rescaling makes each estimate $\bar{M}[t]$ unbiased, as formalized in Theorem 2.

²Each hyperedge is expected to be sampled $\frac{s}{|E|}$ times, and each h-motif instance is counted whenever any of its 3 hyperedges is sampled.

Algorithm 5: MoCHy-A⁺: Approximate H-motif Counting Based on Hyperwedge Sampling

Input : (1) input hypergraph: G = (V, E)(2) projected graph: $\bar{G} = (E, \wedge, \omega)$ (3) number of samples: r**Output:** estimated count of each h-motif t's instances: $\hat{M}[t]$ 1 $M \leftarrow$ map whose default value is 0 2 for $n \leftarrow 1...r$ do $\wedge_{ij} \leftarrow$ a uniformly random hyperwedge з for each hyperedge $e_k \in (N_{e_i} \cup N_{e_j} \setminus \{e_i, e_j\})$ do 4 5 $\hat{M}[h(\{e_i, e_j, e_k\})] += 1$ 6 for each h-motif t do if $17 \leq t \leq 22$ then 7 ▷ open h-motifs $\hat{M}[t] \leftarrow \hat{M}[t] \cdot \frac{|\Lambda|}{2\pi}$ 8 else ▷ closed h-motifs 9 $\hat{M}[t] \leftarrow \hat{M}[t] \cdot \frac{|\wedge|}{3r}$ 10 11 return \hat{M}

Theorem 2 (Bias and Variance of MoCHy-A). For every h-motif t, Algorithm 4 provides an unbiased estimate $\overline{M}[t]$ of the count M[t] of its instances, i.e.,

$$\mathbb{E}[\bar{M}[t]] = M[t]. \tag{4}$$

The variance of the estimate is

$$\operatorname{Var}[\bar{M}[t]] = \frac{1}{3s} \cdot M[t] \cdot (|E| - 3) + \frac{1}{9s} \sum_{l=0}^{2} p_{l}[t] \cdot (l|E| - 9), \quad (5)$$

where $p_l[t]$ is the number of pairs of h-motif t's instances that share l hyperedges.

Proof. See Appendix A.

The time complexity of MoCHy-A is given in Theorem 3.

Theorem 3 (Complexity of MoCHy-A). The average time complexity of Algorithm 4 is $O(\frac{s}{|E|}\sum_{e_i \in E} (|e_i| \cdot |N_{e_i}|^2)).$

Proof. Assume all sets and maps are implemented using hash tables. For a sample hyperedge e_i , computing $N_{e_i} \cup N_{e_j}$ for every $e_j \in N_{e_i}$ takes $O(\sum_{e_j \in N_{e_i}} (|N_{e_i} \cup N_{e_j}|))$ time, and by Lemma 2, computing $h(\{e_i, e_j, e_k\})$ for all considered h-motif instances takes $O(\min(|e_i|, |e_j|) \cdot \sum_{e_j \in N_{e_i}} |N_{e_i} \cup N_{e_j}|)$ time. Thus, from $|N_{e_i} \cup N_{e_j}| \leq |N_{e_i}| + |N_{e_j}|$, the time complexity for processing a sample e_i is

$$\begin{aligned} O(\min(|e_i|, |e_j|) \cdot \sum_{e_j \in N_{e_i}} (|N_{e_i}| + |N_{e_j}|)) \\ &= O(|e_i| \cdot |N_{e_i}|^2 + \sum_{e_j \in N_{e_i}} (|e_j| \cdot |N_{e_j}|)), \end{aligned}$$

which can be written as

$$O(\sum_{e_i \in E} (\mathbb{1}(e_i \text{ is sampled}) \cdot |e_i| \cdot |N_{e_i}|^2) \\ + \sum_{e_j \in E} (\mathbb{1}(e_j \text{ is adjacent to the sample}) \cdot |e_j| \cdot |N_{e_j}|)).$$

From this, linearity of expectation, $\mathbb{E}[\mathbb{1}(e_i \text{ is sampled})] = \frac{1}{|E|}$, and $\mathbb{E}[\mathbb{1}(e_j \text{ is adjacent to the sample})] = \frac{|Ne_j|}{|E|}$, the average time complexity per sample hyperedge becomes $O(\frac{1}{|E|}\sum_{e_i \in E}(|e_i| \cdot |Ne_i|^2))$. Hence, the total time complexity for processing *s* samples is $O(\frac{s}{|E|}\sum_{e_i \in E}(|e_i| \cdot |Ne_i|^2))$.

MoCHy-A⁺: Hyperwedge Sampling (Algorithm 5):

 $MoCHy-A^+$ (Algorithm 5) provides a better trade-off between speed and accuracy than MoCHy-A. Different from MoCHy-A, which samples hyperedges, MoCHy-A⁺ is based on hyperwedge sampling. It selects r hyperwedges uniformly at random with replacement (line 3), and for each sampled hyperwedge $\wedge_{ij} \in \wedge$, it searches for all h-motif instances that contain \wedge_{ij} (lines 4-5). To this end, the hyperedges that are adjacent to e_i or e_j in the projected graph \bar{G} are considered (line 4). For each such instance $\{e_i, e_j, e_k\}$ of h-motif t, the corresponding estimate $\hat{M}[t]$ is incremented (line 5). Lastly, each estimate $\hat{M}[t]$ is rescaled so that it unbiasedly estimates M[t], as formalized in Theorem 4. To this end, it is multiplied by the reciprocal of the expected number of times that each instance of h-motif t is counted.³

Theorem 4 (Bias and Variance of MoCHy-A⁺). For every h-motif t, Algorithm 5 provides an unbiased estimate $\hat{M}[t]$ of the count M[t] of its instances, i.e.,

$$\mathsf{E}[\hat{M}[t]] = M[t]. \tag{6}$$

For every closed h-motif t, the variance of the estimate is

$$\mathbb{V}\mathrm{ar}[\hat{M}[t]] = \frac{1}{3r} \cdot M[t] \cdot (|\wedge| - 3) + \frac{1}{9r} \sum_{n=0}^{1} q_n[t] \cdot (n|\wedge| - 9), \quad (7)$$

where $q_n[t]$ is the number of pairs of h-motif t's instances that share n hyperwedges. For every open h-motif t, the variance is

$$\operatorname{Var}[\hat{M}[t]] = \frac{1}{2r} \cdot M[t] \cdot (|\wedge| - 2) + \frac{1}{4r} \sum_{n=0}^{1} q_n[t] \cdot (n|\wedge| - 4).$$
(8)

The time complexity of $MoCHy-A^+$ is given in Theorem 5.

Theorem 5 (Complexity of MoCHy-A⁺). The average time complexity of Algorithm 5 is $O(\frac{r}{|\wedge|}\sum_{e_i \in E} (|e_i| \cdot |N_{e_i}|^2))$.

Proof. Assume all sets and maps are implemented using hash tables. For a sample hyperwedge \wedge_{ij} , computing $N_{e_i} \cup N_{e_j}$ takes $O(|N_{e_i} \cup N_{e_j}|)$ time, and by Lemma 2, computing $h(\{e_i, e_j, e_k\})$ for all considered h-motif instances takes $O(\min(|e_i|, |e_j|) \cdot |N_{e_i} \cup N_{e_j}|)$ time. Thus, from $|N_{e_i} \cup N_{e_j}| \leq |N_{e_i}| + |N_{e_j}|$, the time complexity for processing a sample \wedge_{ij} is $O(\min(|e_i|, |e_j|) \cdot (|N_{e_i}| + |N_{e_j}|)) = O(|e_i| \cdot |N_{e_i}| + |e_j| \cdot |N_{e_j}|)$, which can be written as

$$O(\sum_{e_i \in E} (\mathbb{1}(e_i \text{ is included in the sample}) \cdot |e_i| \cdot |N_{e_i}|) + \sum_{e_j \in E} (\mathbb{1}(e_j \text{ is included in the sample}) \cdot |e_j| \cdot |N_{e_j}|)).$$

From this, linearity of expectation, $\mathbb{E}[\mathbb{1}(e_i \text{ is included in the sample})] = \frac{|N_{e_i}|}{|\wedge|}$, and $\mathbb{E}[\mathbb{1}(e_j \text{ is included in the sample})] = \frac{|N_{e_i}|}{|\wedge|}$, the average time complexity per sample hyperwedge is $O(\frac{1}{|\wedge|}\sum_{e_i\in E}(|e_i|\cdot|N_{e_i}|^2))$. Hence, the total time complexity for processing r samples is $O(\frac{r}{|\wedge|}\sum_{e_i\in E}(|e_i|\cdot|N_{e_i}|^2))$.

Comparison of MoCHy-A and MoCHy-A⁺: Empirically, MoCHy-A⁺ provides a better trade-off between speed and accuracy than MoCHy-A, as presented in Section 4.5. We provide an analysis that supports this observation. Assume that the numbers of samples in both algorithms are set so ³Note that each instance of open and closed h-motifs contains 2 and 3 hyperwedges, respectively. Each instance of closed h-motifs is counted if one of the 3 hyperwedges in it is sampled, while that of open hmotifs is counted if one of the 2 hyperwedges in it is sampled. Thus, on average, each instance of open and closed h-motifs is counted $3r/|\wedge|$ and $2r/|\wedge|$ times, respectively.

Table 2: Statistics of 11 real hypergraphs from 5 domains.

Dataset	$ V $	E	$ \bar{e} ^*$		# H-motifs
coauth-DBLP coauth-geology coauth-history	$\begin{vmatrix} 1,924,991 \\ 1,256,385 \\ 1,014,734 \end{vmatrix}$	2,466,792 1,203,895 895,439	25 25 25	125M 37.6M 1.7M	$ \begin{vmatrix} 26.3 \text{B} \pm 18 \text{M} \\ 6 \text{B} \pm 4.8 \text{M} \\ 83.2 \text{M} \end{vmatrix} $
contact-primary contact-high	242 327	$12,704 \\ 7,818$	5 5	2.2M 593K	617M 69.7M
email-Enron email-EU	143 998	$1,512 \\ 25,027$	18 25	87.8K 8.3M	9.6M 7B
tags-ubuntu tags-math	$3,029 \\ 1,629$	$147,222 \\ 170,476$	5 5	564M 913M	$4.3T \pm 1.5B$ $9.2T \pm 3.2B$
threads-ubuntu threads-math	$125,602 \\ 176,445$	$166,999 \\ 595,749$	14 21	21.6M 647M	$\begin{vmatrix} 11.4B \\ 2.2T \pm 883M \end{vmatrix}$
* The maximum	size of a hyp	peredge.			

that $\alpha = \frac{s}{|E|} = \frac{r}{|\wedge|}$. For each h-motif t, since both estimates $\overline{M}[t]$ of MoCHy-A and $\widehat{M}[t]$ of MoCHy-A⁺ are unbiased (see Eqs. (4) and (6)), we only need to compare their variances. By Eq. (5), $\operatorname{Var}[\overline{M}[t]] = O(\frac{M[t]+p_1[t]+p_2[t]}{\alpha})$, and by Eq. (7) and Eq. (8), $\operatorname{Var}[\widehat{M}[t]] = O(\frac{M[t]+q_1[t]}{\alpha})$. By definition, $q_1[t] \leq p_2[t]$, and thus $\frac{M[t]+q_1[t]}{\alpha} \leq \frac{M[t]+p_1[t]+p_2[t]}{\alpha}$. Moreover, in real-world hypergraphs, $p_1[t]$ tends to be several orders of magnitude larger than the other terms (i.e., $p_2[t], q_1[t], \text{ and } M[t])$, and thus $\overline{M}[t]$ of MoCHy-A tends to have larger variance (and thus larger estimation error) than $\widehat{M}[t]$ of MoCHy-A⁺. Despite this fact, as shown in Theorems 3 and 5, MoCHy-A and MoCHy-A⁺ have the same time complexity, $O(\alpha \cdot \sum_{e_i \in E} (|e_i| \cdot |N_{e_i}|^2))$. Hence, MoCHy-A⁺ is expected to give a better trade-off between speed and accuracy than MoCHy-A, as confirmed empirically in Section 4.5.

3.4 Parallel and On-the-fly Implementations

We discuss parallelization of MoCHy and then on-the-fly computation of projected graphs.

Parallelization: All versions of MoCHy and hypergraph projection are easily parallelized. Specifically, we can parallelize hypergraph projection and MoCHy-E by letting multiple threads process different hyperedges (in line 3 of Algorithm 1 and line 2 of Algorithm 2) independently in parallel. Similarly, we can parallelize MoCHy-A and MoCHy-A⁺ by letting multiple threads sample and process different hyperedges (in line 3 of Algorithm 4) and hyperwedges (in line 3 of Algorithm 5) independently in parallel. The estimated counts of the same h-motif obtained by different threads are summed up only once before they are returned as outputs. We present some empirical results in Section 4.5.

H-motif Counting without Projected Graphs: If the input hypergraph G is large, computing its projected graph \overline{G} (Algorithm 1) is time and space consuming. Specifically, building G takes $O(\sum_{\bigwedge_{ij} \in \bigwedge} |e_i \cap e_j|)$ time (see Lemma 1) and requires $O(|E| + |\wedge|)$ space, which often exceeds $O(\sum_{e_i \in E}$ $|e_i|$) space required for storing G. Thus, instead of precomputing \overline{G} entirely, we can build it incrementally while memoizing partial results within a given memory budget. For example, in $MoCHy-A^+$ (Algorithm 5), we compute the neighborhood of a hyperedge $e_i \in E$ in \overline{G} (i.e., $\{(k, \omega(\wedge_{ik})) :$ $k \in N_{e_i}$) only if (1) a hyperwedge with e_i (e.g., \wedge_{ij}) is sampled (in line 3) and (2) its neighborhood is not memoized, as described in the pseudocode in Appendix G of [1]. Whether they are computed on the fly or read from memoized results, we always use exact neighborhoods, and thus this change does not affect the accuracy of the considered algorithm.

This incremental computation of \overline{G} can be beneficial in terms of speed since it skips projecting the neighborhood of a hyperedge if no hyperwedge containing it is sampled. However, it can also be harmful if memoized results exceed the memory budget and some parts of \overline{G} need to be rebuilt multiple times. Then, given a memory budget in bits, how should we prioritize hyperedges if all their neighborhoods cannot be memoized? According to our experiments, despite their large size, memoizing the neighborhoods of hyperedges with high degree in \overline{G} makes MoCHy-A⁺ faster than memoizing the neighborhoods of randomly chosen hyperedges or least recently used (LRU) hyperedges. We experimentally examine the effects of the memory budget in Section 4.5.

4. EXPERIMENTS

In this section, we review our experiments that we design for answering the following questions:

- Q1. Comparison with Random: Does counting instances of different h-motifs reveal structural design principles of real-world hypergraphs distinguished from those of random hypergraphs?
- Q2. Comparison across Domains: Do characteristic profiles capture local structural patterns of hypergraphs unique to each domain?
- Q3. Observations and Applications: What are interesting discoveries and applications of h-motifs in realworld hypergraphs?
- Q4. Performance of Counting Algorithms: How fast and accurate are the different versions of MoCHy? Does the advanced version outperform the basic ones?

4.1 Experimental Settings

<u>Machines</u>: We conducted all the experiments on a machine with an AMD Ryzen 9 3900X CPU and 128GB RAM.

Implementations: We implemented all versions of MoCHy using C++ and OpenMP.

Datasets: We used the following eleven real-world hypergraphs from five different domains:

- co-authorship (coauth-DBLP, coauth-geology [58], and coauth-history [58]): A node represents an author. A hyperedge represents all authors of a publication.
- contact (contact-primary [59] and contact-high [44]): A node represents a person. A hyperedge represents a group interaction among individuals.
- email (email-Enron [37] and email-EU [40, 68]): A node represents an e-mail account. A hyperedge consists of the sender and all receivers of an email.
- tags (tags-ubuntu and tags-math): A node represents a tag. A hyperedge represents all tags attached to a post.
- threads (threads-ubuntu and threads-math): A node represents a user. A hyperedge groups all users participating in a thread.

These hypergraphs are made public by the authors of [12], and in Table 2 we provide some statistics of the hypergraphs after removing duplicated hyperedges. We used MoCHy-E for the *coauth-history* dataset, the *threads-ubuntu* dataset, and all datasets from the **contact** and **email** domains. For the other datasets, we used MoCHy-A⁺ with r = 2,000,000, unless otherwise stated. We used a single thread unless otherwise stated. We computed CPs based on five hypergraphs randomized as described in Section 2.2.

Table 3: Real-world and random hypergraphs have distinct distributions of h-motif instances. We report the absolute counts of each h-motif's instances in a real-world hypergraph from each domain and its corresponding random hypergraph. To compare the counts in both hypergraphs, we measure the relative count (RC) of each h-motif. We also rank the counts, and we report each h-motif's rank difference (RD) in the real-world and corresponding random hypergraphs.

							-						-							
îf	co	auth-DBL	P		con	tact-prima	ary	-		email-EU			t	ags-math	-		th	reads-mat	h	
h-motif	count	(rank)	RD	RC	count	(rank)	RD	RC	count	(rank)	RD	RC	count	(rank)	RD	RC	count	(rank)	RD	RC
ż	real	random	КD	i to	real	random	ΝĐ	i to	real	random	ιτυ	i to	real	random	ΝD	i to	real	random	ΝD	i to
1	9.6E07 (7)	1.3E09 (4)	3	-0.86	4.8E04 (16)	2.8E07 (5)	11	-1.00	7.5E06 (13)	1.7E08 (7)	6	-0.91	9.0E08 (13)	2.2E11 (6)	7	-0.99	6.4E08 (7)	2.4E11 (4)	3	-0.99
2	7.0E09 (2)	7.2E09 (2)	0	-0.01	1.1E08 (3)	8.6E07 (3)	0	0.12	6.3E08 (2)	8.2E08 (3)	1	-0.13	1.6E12 (<mark>2</mark>)	1.6E12 (<mark>2</mark>)	0	0.02	1.1E12 (<mark>2</mark>)	7.7E11 (2)	0	0.16
3	2.2E06 (17)	6.1E03 (<mark>14</mark>)	3	0.99	2.8E03 (21)	1.7E05 (16)	5	-0.97	1.6E06 (21)	7.8E05 (17)	4	0.34	3.0E06 (20)	1.1E09 (15)	5	-0.99	1.7E05 (20)	1.7E08 (14)	6	-1.00
4	9.6E06 (11)	1.1E05 (12)	1	0.98	8.4E02 (24)	9.2E05 (12)	12	-1.00	4.3E06 (<mark>16</mark>)	1.5E07 (12)	4	-0.55	1.5E08 (17)	1.6E10 (12)	5	-0.98	3.1E06 (<mark>13</mark>)	1.2E09 (11)	2	-0.99
5	1.5E08 (6)	1.2E05 (11)	5	1.00	4.6E06 (5)	1.6E06 (11)	6	0.49	7.5E07 (<mark>7</mark>)	1.1E07 (13)	6	0.74	7.4E09 (<mark>8</mark>)	2.5E10 (<mark>8</mark>)	0	-0.54	4.1E08 (<mark>8</mark>)	1.7E09 (10)	2	-0.61
6	9.9E08 (3)	1.8E06 (<mark>9</mark>)	6	1.00	1.3E07 (4)	8.2E06 (7)	3	0.24	3.9E08 (4)	1.9E08 (<mark>6</mark>)	2	0.34	6.8E11 (<mark>3</mark>)	3.3E11 (4)	1	0.35	1.4E10 (4)	1.1E10 (<mark>8</mark>)	4	0.11
7	1.9E05 (23)	0.0E00 (<mark>20</mark>)	3	1.00	1.6E04 (17)	2.0E02 (24)	7	0.98	7.5E04 (<mark>24</mark>)	1.2E02 (<mark>25</mark>)	1	1.00	8.3E05 (<mark>25</mark>)	9.1E05 (<mark>25</mark>)	0	-0.05	8.8E03 (<mark>24</mark>)	1.7E04 (24)	0	-0.32
8	3.9E05 (22)	0.0E00 (<mark>20</mark>)	2	1.00	4.6E03 (20)	2.6E03 (22)	2	0.27	4.2E06 (17)	2.5E04 (21)	4	0.99	2.0E06 (23)	3.4E07 (22)	1	-0.89	2.2E04 (23)	3.5E05 (21)	2	-0.88
9	2.4E06 (16)	0.0E00 (<mark>20</mark>)	4	1.00	1.7E05 (12)	4.6E03 (20)	8	0.95	1.8E06 (<mark>20</mark>)	1.1E04 (22)	2	0.99	1.4E08 (<mark>18</mark>)	5.4E07 (21)	3	0.45	5.1E05 (17)	4.5E05 (20)	3	0.06
10	7.6E06 (13)	7.5E00 (18)	5	1.00	5.7E04 (15)	5.5E04 (17)	2	0.03	2.8E07 (10)	1.7E06 (14)	4	0.88	7.1E08 (<mark>14</mark>)	1.9E09 (14)	0	-0.45	2.3E06 (15)	9.4E06 (17)	2	-0.61
11	8.6E06 (12)	0.9E00 (<mark>19</mark>)	7	1.00	4.1E05 (11)	2.4E04 (18)	7	0.89	9.0E06 (11)	1.9E05 (19)	8	0.96	3.5E09 (<mark>10</mark>)	7.4E08 (16)	6	0.65	2.8E06 (14)	3.1E06 (18)	4	-0.05
12	6.4E07 (<mark>8</mark>)	1.9E02 (16)	8	1.00	1.7E05 (13)	2.7E05 (14)	1	-0.24	8.2E07 (<mark>6</mark>)	2.4E07 (10)	4	0.55	6.9E10 (<mark>6</mark>)	2.4E10 (10)	4	0.49	8.2E07 (<mark>10</mark>)	6.2E07 (15)	5	0.14
13	1.6E04 (26)	0.0E00 (<mark>20</mark>)	6	1.00	5.5E03 (19)	1.6E00 (26)	7	1.00	2.7E04 (26)	0.4E00 (26)	0	1.00	1.1E06 (<mark>24</mark>)	1.7E04 (26)	2	0.97	1.5E02 (<mark>26</mark>)	8.6E00 (26)	0	0.89
14	1.4E05 (24)	0.0E00 (<mark>20</mark>)	4	1.00	6.0E03 (18)	7.1E01 (25)	7	0.98	7.2E05 (22)	3.7E02 (24)	2	1.00	2.8E07 (19)	1.8E06 (24)	5	0.88	3.9E03 (25)	9.3E02 (25)	0	0.61
15	6.5E05 (19)	0.0E00 (<mark>20</mark>)	1	1.00	1.7E03 (22)	8.6E02 (23)	1	0.34	3.6E06 (19)	5.0E04 (20)	1	0.97	2.9E08 (15)	5.7E07 (20)	5	0.67	2.7E04 (<mark>22</mark>)	2.0E04 (23)	1	0.16
16	2.0E06 (18)	0.0E00 (<mark>20</mark>)	2	1.00	1.4E02 (25)	3.2E03 (21)	4	-0.92	6.7E06 (14)	1.7E06 (15)	1	0.60	1.9E09 (<mark>11</mark>)	5.8E08 (18)	7	0.53	2.4E05 (<mark>18</mark>)	1.3E05 (22)	4	0.29
17	4.2E05 (21)	2.0E06 (<mark>8</mark>)	13	-0.65	1.0E03 (23)	6.3E05 (13)	10	-1.00	3.8E04 (<mark>25</mark>)	8.7E05 (16)	9	-0.92	5.1E05 (<mark>26</mark>)	5.0E08 (19)	7	-1.00	2.3E05 (<mark>19</mark>)	9.2E08 (12)	7	-1.00
18	2.6E06 (15)	6.4E07 (7)	8	-0.92	1.2E02 (26)	7.0E06 (8)	18	-1.00	6.0E06 (15)	4.0E07 (8)	7	-0.74	2.5E06 (<mark>22</mark>)	1.6E10 (13)	9	-1.00	8.3E05 (16)	1.3E10 (7)	9	-1.00
19	3.6E07 (9)	6.7E07 (<mark>6</mark>)	3	-0.30	2.0E06 (6)	1.2E07 (6)	0	-0.72	8.7E06 (12)	2.9E07 (<mark>9</mark>)	3	-0.54	9.4E08 (12)	2.4E10 (9)	3	-0.93	3.5E08 (<mark>9</mark>)	1.8E10 (6)	3	-0.96
20	3.4E08 (5)	2.2E09 (3)	2	-0.73	6.0E05 (10)	1.3E08 (2)	8	-0.99	2.2E08 (5)	1.2E09 (<mark>2</mark>)	3	-0.69	9.2E09 (7)	7.2E11 (3)	4	-0.97	1.9E09 (<mark>5</mark>)	2.4E11 (3)	2	-0.98
21	7.9E08 (4)	5.6E08 (<mark>5</mark>)	1	0.17	1.7E08 (2)	5.7E07 (4)	2	0.50	5.3E08 (<mark>3</mark>)	2.3E08 (4)	1	0.39	1.2E11 (<mark>5</mark>)	2.8E11 (5)	0	-0.40	2.8E10 (<mark>3</mark>)	8.6E10 (5)	2	-0.51
22	1.7E10 (1)	1.8E10 (1)	0	-0.03	3.1E08 (1)	5.8E08 (1)	0	-0.30	4.9E09 (1)	8.5E09 (1)	0	-0.27	6.6E12 (1)	7.6E12 (1)	0	-0.07	1.1E12 (1)	1.2E12 (1)	0	-0.02
23	2.4E04 (25)	1.5E01 (17)	8	1.00	1.2E05 (14)	5.4E03 (19)	5	0.91	8.8E04 (23)	4.0E03 (23)	0	0.91	2.6E06 (<mark>21</mark>)	7.9E06 (23)	2	-0.51	1.4E05 (<mark>21</mark>)	7.8E05 (19)	2	-0.70
24	4.4E05 (20)	1.4E03 (15)	5	0.99	7.7E05 (9)	1.8E05 (15)	6	0.63	4.2E06 (18)	5.4E05 (18)	0	0.77	2.2E08 (16)	7.2E08 (17)	1	-0.53	7.5E06 (12)	3.1E07 (16)	4	-0.61
25	3.8E06 (14)	4.6E04 (13)	1	0.98	1.7E06 (8)	1.8E06 (10)	2	-0.03	3.2E07 (9)	2.0E07 (11)	2	0.23	6.0E09 (<mark>9</mark>)	2.0E10 (11)	2	-0.54	8.0E07 (11)	4.2E08 (13)	2	-0.68
26	2.3E07 (10)	4.9E05 (10)	0	0.96	1.8E06 (7)	6.14E06 (9)	2	-0.54	7.5E07 (8)	2.1E08 (5)	3	-0.48	1.3E11 (4)	1.8E11 (7)	3	-0.14	1.2E09 (6)	1.9E09 (9)	3	-0.21
-	• • • • •	, .,			• • • /						-		/	· · · · ·	_		/		_	_

4.2 Q1. Comparison with Random

We analyze the counts of different h-motifs' instances in real and random hypergraphs. In Table 3, we report the (approximated) count of each h-motif t's instances in each real hypergraph with the corresponding count averaged over five random hypergraphs obtained as described in Section 2.2. For each h-motif t, we measure its relative count, which we define as $\frac{M[t]-M_{rand}[t]}{M[t]+M_{rand}[t]}$. We also rank h-motifs by the counts of their instances and examine the difference between the ranks in real and corresponding random hypergraphs. As seen in the table, the count distributions in real hypergraphs are clearly distinguished from those of random hypergraphs. H-motifs in Random Hypergraphs: We notice that instances of h-motifs 17 and 18 appear much more frequently in random hypergraphs than in real hypergraphs from all domains. For example, instances of h-motif 17 appear only about 510 thousand times in the tags-math dataset, while they appear about 500 million times (about $980 \times$ more often) in the corresponding randomized hypergraph. In the threads-math dataset, instances of h-motif 18 appear about 830 thousand times, while they appear about 13 billion times (about $15,660 \times$ more often) in the corresponding randomized hypergraph. Instances of h-motifs 17 and 18 consist of a hyperedge and its two disjoint subsets (see Figure 3).

H-motifs in Co-authorship Hypergraphs: We observe that instances of h-motifs 10, 11 and 12 appear more frequently in all three hypergraphs from the **co-authorship** domain than in the corresponding random hypergraphs. Although there are only about 190 instances of h-motif 12 in the corresponding random hypergraphs, there are about 64 million such instances (about **337**, **000**× more instances) in the *coauth-DBLP* dataset. As seen in Figure 3, in instances of h-motifs 10, 11, and 12, a hyperedge is overlapped with the two other overlapped hyperedges in three different ways.

H-motifs in Contact Hypergraphs: Instances of h-motifs 9, 13, and 14 are noticeably more common in both **contact** datasets than in the corresponding random hypergraphs. As seen in Figure 3, in instances of h-motifs 9, 13 and 14, hyperedges are tightly connected and nodes are mainly located in the intersections of all or some hyperedges. **H-motifs in Email Hypergraphs:** Both email datasets contain particularly many instances of h-motifs 8 and 10, compared to the corresponding random hypergraphs. As seen in Figure 3, instances of h-motifs 8 and 10 consist of three hyperedges one of which contains most nodes.

H-motifs in Tags Hypergraphs: In addition to instances of h-motif 11, which are common in most real hypergraphs, instances of h-motif 16, where all seven regions are not empty (see Figure 3), are particularly frequent in both tags datasets than in corresponding random hypergraphs.

<u>H-motifs in Threads Hypergraphs:</u> Lastly, in both data sets from the **threads** domain, instances of h-motifs 12 and 24 are noticeably more frequent than expected from the corresponding random hypergraphs.

In Appendix C.1 of [1], we analyze how the significance of each h-motif and the rank difference for it are related to global structural properties of hypergraphs.

4.3 Q2. Comparison across Domains

We compare the characteristic profiles (CPs) of the realworld hypergraphs. In Figure 5, we present the CPs (i.e., the significances of the 26 h-motifs) of each hypergraph. As seen in the figure, hypergraphs from the same domains have similar CPs. Specifically, all three hypergraphs from the **co-authorship** domain share extremely similar CPs, even when the absolute counts of h-motifs in them are several orders of magnitude different. Similarly, the CPs of both hypergraphs from the **tags** domain are extremely similar. However, the CPs of the three hypergraphs from the

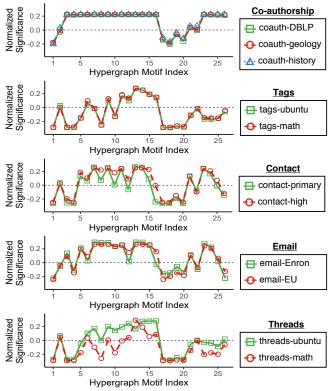
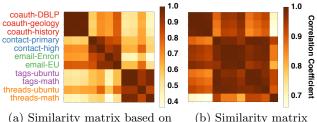


Figure 5: Characteristic profiles (CPs) capture local structural patterns of real-world hypergraphs accurately. The CPs are similar within domains but different across domains. Note that the significance of h-motif 3 distinguishes the contact hypergraphs from the email hypergraphs.



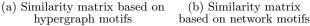


Figure 6: Characteristic profiles (CPs) based on hypergraph motifs (h-motifs) capture local structural patterns more accurately than CPs based on network motifs. The CPs based on h-motifs distinguishes the domains of the real-world hypergraphs better than the CPs based on network motifs.

co-authorship domain are clearly distinguished by them of the hypergraphs from the tags domain. While the CPs of the hypergraphs from the contact domain and the CPs of those from the email domain are similar for the most part, they are distinguished by the significance of h-motif 3. These observations confirm that CPs accurately capture local structural patterns of real-world hypergraphs. In Appendix C.2 of [1], we analyze the importance of each h-motif in terms its contribution to distinguishing the domains.

To further verify the effectiveness of CPs based on hmotifs, we compare them with CPs based on network motifs. Specifically, we represent each hypergraph G = (V, E)as a bipartite graph G' = (V', E') where $V' := V \cup E$ and $E' := \{(v, e) \in V \times E : v \in e\}$, which is also known as *star expansion* [60]. That is, the two types of nodes in the transformed bipartite graph G' represent the nodes and hy-

Table 4: H-motifs give informative features. Using them in HM26 or HM7 yields more accurate hyperedge predictions than using the baseline features in HC.

		HM26	$\mathbf{HM7}$	\mathbf{HC}
Logistic Regression	$\begin{array}{c} \mathbf{ACC}*\\ \mathbf{AUC}\dagger \end{array}$	$0.754 \\ 0.813$	$0.656 \\ 0.693$	$0.636 \\ 0.691$
Random Forest	ACC AUC	$0.768 \\ 0.852$	$0.741 \\ 0.779$	$0.639 \\ 0.692$
Decision Tree	ACC AUC	$\begin{array}{c} 0.731 \\ 0.732 \end{array}$	$0.684 \\ 0.685$	$0.613 \\ 0.616$
K-Nearest Neighbors	ACC AUC	$0.694 \\ 0.750$	$0.689 \\ 0.743$	$0.640 \\ 0.684$
MLP Classifier	ACC AUC	$0.795 \\ 0.875$	$0.762 \\ 0.841$	$0.646 \\ 0.701$

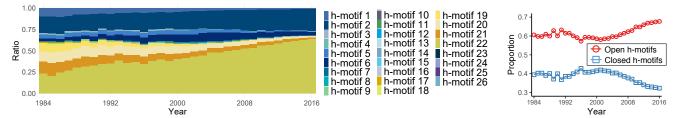
peredges, respectively, in the original hypergraph G, and each edge (v, e) in G' indicates that the node v belongs to the hyperedge e in G. Then, we compute the CPs based on the network motifs consisting of 3 to 5 nodes, using [18]. Lastly, based on both CPs, we compute the similarity matrices (specifically, correlation coefficient matrices) of the real-world hypergraphs. As seen in Figure 6, the domains of the real-world hypergraphs are distinguished more clearly by the CPs based on h-motifs than by the CPs based on network motifs. Numerically, when the CPs based on h-motifs are used, the average correlation coefficient is 0.978 within domains and 0.654 across domains, and the gap is 0.324. However, when the CPs based on network motifs are used, the average correlation coefficient is 0.988 within domains and 0.919 across domains, and the gap is just 0.069. These results support that h-motifs play a key role in capturing local structural patterns of real-world hypergraphs.

4.4 Q3. Observations and Applications

We conduct two case studies on the *coauth-DBLP* dataset, which is a **co-authorship** hypergraph.

Evolution of Co-authorship Hypergraphs: The dataset contains bibliographic information of computer science publications. Using the publications in each year from 1984 to 2016, we create 33 hypergraphs where each node corresponds to an author, and each hyperedge indicates the set of the authors of a publication. Then, we compute the fraction of the instances of each h-motif in each hypergraph to analyze patterns and trends in the formation of collaborations. As shown in Figure 7, over the 33 years, the fractions have changed with distinct trends. First, as seen in Figure 7(b), the fraction of the instances of open h-motifs has increased steadily since 2001, indicating that collaborations have become less clustered, i.e., the probability that two collaborations intersecting with a collaboration also intersect with each other has decreased. Notably, the fractions of the instances of h-motif 2 (closed) and h-motif 22 (open) have increased rapidly, accounting for most of the instances. Hyperedge Prediction: As an application of h-motifs, we

consider the problem of predicting publications (i.e., hyperedges) in 2016 based on the publications from 2013 to 2015. As in [69], we formulate this problem as a binary classification problem where we aim to classify real hyperedges and fake ones. To this end, we create fake hyperedges in both training and test sets by replacing some fraction of nodes in each real hyperedge with random nodes (see Appendix E of [1] for details). Then, we train five classifiers using the following three different sets of input hyperedge features:



(a) Fraction of the instances of each h-motif in the coauth-DBLP dataset over time. (b) Open and closed h-motifs. Figure 7: Trends in the formation of collaborations are captured by h-motifs. (a) The fractions of the instances of h-motifs 2 and 22 have increased rapidly. (b) The fraction of the instances of open h-motifs has increased steadily since 2001.

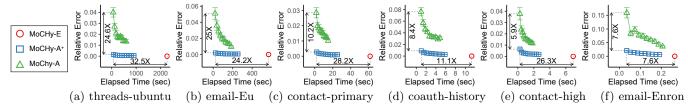


Figure 8: MoCHy-A⁺ gives the best trade-off between speed and accuracy. It yields up to $25 \times$ more accurate estimation than MoCHy-A, and it is up to $32.5 \times$ faster than MoCHy-E. The error bars indicate ± 1 standard error over 20 trials.

- HM26 (∈ ℝ²⁶): The number of each h-motif's instances that contain each hyperedge.
- HM7 (∈ ℝ⁷): The seven features with the largest variance among those in HM26.
- HC (∈ ℝ⁷): The mean, maximum, and minimum degree⁴ and the mean, maximum, and minimum number of neighbors⁵ of the nodes in each hyperedge and its size.

We report the accuracy (ACC) and the area under the ROC curve (AUC) in each setting in Table 4. Using **HM7**, which is based on h-motifs, yields consistently better predictions than using an equal number of baseline features in **HC**. Using **HM26** yields the best predictions. These results indicate informative features can be obtained from h-motifs.

4.5 Q4. Performance of Counting Algorithms

We test the speed and accuracy of all versions of MoCHy under various settings. To this end, we measure elapsed time and relative error defined as

$$\frac{\sum_{t=1}^{26} |M[t] - \bar{M}[t]|}{\sum_{t=1}^{26} M[t]} \text{ and } \frac{\sum_{t=1}^{26} |M[t] - \hat{M}[t]|}{\sum_{t=1}^{26} M[t]}$$

for MoCHy-A and MoCHy-A⁺, respectively.

Speed and Accuracy: In Figure 8, we report the elapsed time and relative error of all versions of MoCHy on the 6 different datasets where MoCHy-E terminates within a reasonable time. The numbers of samples in MoCHy-A and MoCHy-A⁺ are set to $\{2.5 \times k : 1 \leq k \leq 10\}$ percent of the counts of hyperedges and hyperwedges, respectively. MoCHy-A⁺ provides the best trade-off between speed and accuracy. For example, in the threads-ubuntu dataset, MoCHy- A^+ provides 24.6× lower relative error than MoCHy-A, consistently with our theoretical analysis (see the last paragraph of Section 3.3). Moreover, in the same dataset, $MoCHv-A^+$ is $32.5 \times$ faster than MoCHy-E with little sacrifice on accuracy. Effects of the Sample Size on CPs: In Figure 9, we report the CPs obtained by $MoCHy-A^+$ with different numbers ⁴The degree of a node v is the number of hyperedges that contain v. 5 The neighbors of a node v is the nodes that appear in at least one hyperedge together with v.

of hyperwedge samples on 3 datasets. Even with a smaller number of samples, the CPs are estimated near perfectly.

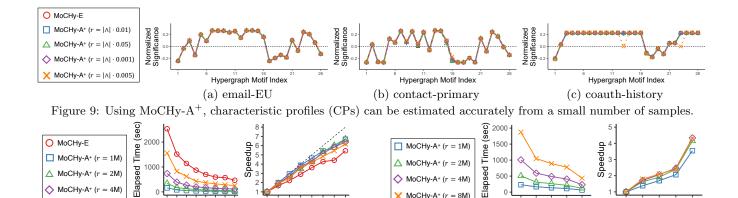
Parallelization: We measure the running times of MoCHy-E and MoCHy-A⁺ with different numbers of threads on the *threads-ubuntu* dataset. As seen in Figure 10, both algorithms achieve significant speedups with multiple threads. Specifically, with 8 threads, MoCHy-E and MoCHy-A⁺ (r = 1M) achieve speedups of 5.4 and 6.7, respectively.

Effects of On-the-fly Computation on Speed: We analyze the effects of the on-the-fly computation of projected graphs (discussed in Section 3.4) on the speed of $MoCHy-A^+$ under different memory budgets for memoization. To this end, we use the *threads-ubuntu* dataset, and we set the memory budgets so that up to {0%, 0.1%, 1%, 10%, 100%} of the edges in the projected graph can be memoized. The results are shown in Figure 11. As the memory budget increases, MoCHy-A⁺ becomes faster, avoiding repeated computation. Due to our careful prioritization scheme based on degree, memoizing 1% of the edges achieves speedups of about 2.

5. RELATED WORK

We review prior work on network motifs, algorithms for counting them, and hypergraphs. While the definition of a network motif varies among studies, here we define it as a connected graph composed by a predefined number of nodes. Network Motifs. Network motifs were proposed as a tool for understanding the underlying design principles and capturing the local structural patterns of graphs [26, 55, 46]. The occurrences of motifs in real-world graphs are significantly different from those in random graphs [46], and they vary also depending on the domains of graphs [45]. The concept of network motifs has been extended to various types of graphs, including dynamic [49], bipartite [16], and heterogeneous [51] graphs. The occurrences of network motifs have been used in a wide range of graph applications: community detection [13, 68, 43, 62], ranking [73], graph embedding [52, 71], and graph neural networks [39], to name a few.

Algorithms for Network Motif Counting. We focus on algorithms for counting the occurrences of every network motif whose size is fixed or within a certain range [4, 5, 9, 18, 21, 25, 50], while many are for a specific motif (e.g., the



3 4 5 6 7

Number of Threads Number of Threads (a) Elapsed Time (b) Speedup Figure 10: Both MoCHy-E and MoCHy-A⁺ achieve significant speedups with multiple threads.

5678

= 4M)

MoCHy-A⁺ (r = 8M)

clique of size 3) [3, 22, 27, 28, 31, 36, 38, 48, 54, 56, 57, 61, 63, 65]. Given a graph, they aim to count rapidly and accurately the instances of motifs with 4 or more nodes, despite the combinatorial explosion of the instances, using the following techniques:

- (1) **Combinatorics:** For exact counting, [4, 50, 49] employ combinatorial relations between counts. That is, they deduce the counts of the instances of motifs from those of other smaller or equal-size motifs.
- (2) MCMC: Most approximate algorithms sample motif instances from which they estimate the counts. Employed MCMC sampling, [15, 21, 25, 53, 64] perform a random walk over instances (i.e, connected subgraphs) until it reaches the stationarity to sample an instance from a fixed probability distribution (e.g., uniform).
- (3) Color Coding: Instead of MCMC, [17, 18] employ color coding [7]. Specifically, they color each node uniformly at random among k colors, count the number of k-trees with k colors rooted at each node, and use them to sample instances from a fixed probability distribution.

In our problem, which focuses on h-motifs with only 3 hyperedges, sampling instances with fixed probabilities is straightforward without (2) or (3), and the combinatorial relations on graphs in (1) are not applicable. In algorithmic aspects, we address the computational challenges discussed at the beginning of Section 3 by answering (a) what to precompute (Section 3.1), (b) how to leverage it (Sections 3.2 and 3.3), and (c) how to prioritize it (Sections 3.4 and 4.5), with formal analyses (Lemma 2; Theorems 1, 3, and 5).

Hypergraph. Hypergraphs naturally represent group interactions occurring in a wide range of fields, including computer vision [29, 70], bioinformatics [30], circuit design [34, 47], social network analysis [41, 67], and recommender systems [19, 42]. There also has been considerable attention on machine learning on hypergraphs, including clustering [2, 8, 35, 74], classification [32, 60, 70] and hyperedge prediction [12, 69, 72]. Recent studies on real-world hypergraphs revealed interesting patterns commonly observed across domains, including global structural properties (e.g., giant connected components and small diameter) [23] and temporal patterns regarding arrivals of the same or similar hyperedges [14]. Notably, Benson et al. [12] studied how several local features, including edge density, average degree, and

Figure 11: Memoizing a small fraction of projected graphs leads to significant speedups of MoCHy-A⁺.

Memory (% of Edges) (a) Elapsed Time

10 100

01

10 100

Memory (% of Edges)

(b) Speedup

0.1

probabilities of simplicial closure events for 4 or less nodes⁶. differ across domains. Our analysis using h-motifs is complementary to these approaches in that it (1) captures local patterns systematically without hand-crafted features, (2) captures static patterns without relying on temporal information, and (3) naturally uses hyperedges with any number of nodes without decomposing them into small ones.

CONCLUSIONS 6.

MoCHy-A⁺ (r = 8M)

In this work, we introduce hypergraph motifs (h-motifs), and using them, we investigate the local structures of 11 realworld hypergraphs from 5 different domains. We summarize our contributions as follows:

- Novel Concepts: We define 26 h-motifs, which describe connectivity patterns of three connected hyperedges in a unique and exhaustive way, independently of the sizes of hyperedges (Figure 3).
- Fast and Provable Algorithms: We propose 3 parallel algorithms for (approximately) counting every h-motif's instances, and we theoretically and empirically analyze their speed and accuracy. Both approximate algorithms vield unbiased estimates (Theorems 2 and 4), and especially the advanced one is up to $32 \times$ faster than the exact algorithm, with little sacrifice on accuracy (Figure 8).
- **Discoveries in** 11 **Real-world Hypergraphs:** We confirm the efficacy of h-motifs by showing that local structural patterns captured by them are similar within domains but different across domains (Figures 5 and 6).

Reproducibility: The code and datasets used in this work are available at https://github.com/geonlee0325/MoCHy.

Future directions include extending h-motifs to rich hypergraphs, such as temporal or heterogeneous hypergraphs, and incorporating h-motifs into various tasks, such as hypergraph embedding, ranking, and clustering.

Acknowledgements. This work was supported by National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. NRF-2020R1C1C1008296). This work was also supported by Institute of Information & Communications Technology Planning & Evaluation (IITP) grant funded by the Korea government (MSIT) (No. 2019-0-00075, Artificial Intelligence Graduate School Program (KAIST)) and supported by the National Supercomputing Center with supercomputing resources including technical support (KSC-2020-INO-0004).

⁶The emergence of the first hyperedge that includes a set of nodes each of whose pairs co-appear in previous hyperedges. The configuration of the pairwise co-appearances affects the probability.

APPENDIX A. PROOF OF THEOREM 2

We let $X_{ij}[t]$ be a random variable indicating whether the *i*-th sampled hyperedge (in line 3 of Algorithm 4) is included in the *j*-th instance of h-motif *t* or not. That is, $X_{ij}[t] = 1$ if the hyperedge is included in the instance, and $X_{ij}[t] = 0$ otherwise. We let $\bar{m}[t]$ be the number of times that h-motif *t*'s instances are counted while processing *s* sampled hyperedges. That is,

$$\bar{m}[t] := \sum_{i=1}^{s} \sum_{j=1}^{M[t]} X_{ij}[t].$$
(9)

Then, by lines 8-9 of Algorithm 4,

$$\bar{M}[t] = \bar{m}[t] \cdot \frac{|E|}{3s}.$$
(10)

Proof of the Bias of $\overline{M}[t]$ (Eq. (4)): Since each h-motif instance contains three hyperedges, the probability that each *i*-th sampled hyperedge is contained in each *j*-th instance of h-motif *t* is

$$P[X_{ij}[t] = 1] = \mathbb{E}[X_{ij}[t]] = \frac{3}{|E|}.$$
 (11)

From linearity of expectation,

$$\mathbb{E}[\bar{m}[t]] = \sum_{i=1}^{s} \sum_{j=1}^{M[t]} \mathbb{E}[X_{ij}[t]] = \sum_{i=1}^{s} \sum_{j=1}^{M[t]} \frac{3}{|E|} = \frac{3s \cdot M[t]}{|E|}.$$

Then, by Eq. (10),
$$\mathbb{E}[M[t]] = \frac{|\Sigma|}{3s} \cdot \mathbb{E}[\tilde{m}[t]] = M[t].$$

Proof of the Variance of $\overline{M}[t]$ (Eq. (5)): From Eq. (11) and $X_{ij}[t] = X_{ij}[t]^2$, the variance of $X_{ij}[t]$ is

$$\mathbb{V}\mathrm{ar}[X_{ij}[t]] = \mathbb{E}[X_{ij}[t]^2] - \mathbb{E}[X_{ij}[t]]^2 = \frac{3}{|E|} - \frac{9}{|E|^2}.$$
 (12)

Consider the covariance between $X_{ij}[t]$ and $X_{i'j'}[t]$. If i = i', then from Eq. (11),

$$Cov(X_{ij}[t], X_{i'j'}[t]) = \mathbb{E}[X_{ij}[t] \cdot X_{ij'}[t]] - \mathbb{E}[X_{ij}[t]]\mathbb{E}[X_{ij'}[t]]$$

= $P[X_{ij}[t] = 1, X_{ij'}[t] = 1] - \mathbb{E}[X_{ij}[t]]\mathbb{E}[X_{ij'}[t]]$
= $P[X_{ij}[t] = 1] \cdot P[X_{ij'}[t] = 1|X_{ij}[t] = 1]$
 $- \mathbb{E}[X_{ij}[t]]\mathbb{E}[X_{ij'}[t]]$
= $\frac{3}{|E|} \cdot \frac{l_{jj'}}{3} - \frac{9}{|E|^2} = \frac{l_{jj'}}{|E|} - \frac{9}{|E|^2},$ (13)

where $l_{jj'}$ is the number of hyperedges that the *j*-th and j'-th instances share. However, since hyperedges are sampled independently (specifically, uniformly at random with replacement), if $i \neq i'$, then $Cov(X_{ij}[t], X_{i'j'}[t]) = 0$. This observation, Eq. (9), Eq. (12), and Eq. (13) imply

$$\begin{aligned} & \mathbb{V}\mathrm{ar}[\bar{m}[t]] = \mathbb{V}\mathrm{ar}[\sum_{i=1}^{s} \sum_{j=1}^{M[t]} X_{ij}[t]] \\ &= \sum_{i=1}^{s} \sum_{j=1}^{M[t]} \mathbb{V}\mathrm{ar}[X_{ij}[t]] + \sum_{i=1}^{s} \sum_{j \neq j'} \mathbb{C}\mathrm{ov}(X_{ij}[t], X_{ij'}[t]) \\ &= s \cdot M[t] \cdot (\frac{3}{|E|} - \frac{9}{|E|^2}) + s \sum_{l=0}^{2} p_l[t](\frac{l}{|E|} - \frac{9}{|E|^2}), \end{aligned}$$

where $p_l[t]$ is the number of pairs of h-motif t's instances sharing l hyperedges. This and Eq. (10) imply Eq. (5). \Box

B. PROOF OF THEOREM 4

A random variable $Y_{ij}[t]$ denotes whether the *i*-th sampled hyperwedge (in line 3 of Algorithm 5) is included in

the *j*-th instance of h-motif *t*. That is, $Y_{ij}[t] = 1$ if the sampled hyperwedge is included in the instance, and $Y_{ij}[t] = 0$ otherwise. We let $\hat{m}[t]$ be the number of times that h-motif *t*' instances are counted while processing *r* sampled hyperwedges. That is,

$$\hat{m}[t] := \sum_{i=1}^{r} \sum_{j=1}^{M[t]} Y_{ij}[t]$$
(14)

We use w[t] to denote the number of hyperwedges included in each instance of h-motif t. That is,

$$w[t] := \begin{cases} 2 & \text{if h-motif } t \text{ is open,} \\ 3 & \text{if h-motif } t \text{ is closed.} \end{cases}$$
(15)

Then, by lines 6-10 of Algorithm 5,

$$\hat{M}[t] = \hat{m}[t] \cdot \frac{1}{w[t]} \cdot \frac{|\wedge|}{r}.$$
(16)

Proof of the Bias of $\hat{M}[t]$ (Eq. (6)): Since each instance of h-motif t contains w[t] hyperwedges, the probability that each *i*-th sampled hyperwedge is contained in each *j*-th instance of h-motif t is

$$P[Y_{ij}[t] = 1] = \mathbb{E}[Y_{ij}[t]] = \frac{w[t]}{|\wedge|}.$$
(17)

From linearity of expectation,

$$\mathbb{E}[\hat{m}[t]] = \sum_{i=1}^{r} \sum_{j=1}^{M[t]} \mathbb{E}[Y_{ij}[t]] = \sum_{i=1}^{r} \sum_{j=1}^{M[t]} \frac{w[t]}{|\wedge|} = \frac{w[t] \cdot r \cdot M[t]}{|\wedge|}.$$

Then, by Eq. (16), $\mathbb{E}[\hat{M}[t]] = \mathbb{E}[\hat{m}[t]] \cdot \frac{1}{w[t]} \cdot \frac{|\wedge|}{r} = M[t].$

Proof of the Variance of $\hat{M}[t]$ (Eq. (7) and Eq. (8):

From Eq. (17) and $Y_{ij}[t] = Y_{ij}[t]^2$, the variance of each random variable $Y_{ij}[t]$ is

$$\mathbb{V}\mathrm{ar}[Y_{ij}[t]] = \mathbb{E}[Y_{ij}[t]^2] - \mathbb{E}[Y_{ij}[t]]^2 = \frac{w[t]}{|\wedge|} - \frac{w[t]^2}{|\wedge|^2}.$$
 (18)

Consider the covariance between $Y_{ij}[t]$ and $Y_{i'j'}[t]$. If i = i', then from Eq. (17),

$$\begin{aligned}
& \mathbb{C}\mathrm{ov}(Y_{ij}[t], Y_{i'j'}[t]) = \mathbb{E}[Y_{ij}[t] \cdot Y_{ij'}[t]] - \mathbb{E}[Y_{ij}[t]]\mathbb{E}[Y_{ij'}[t]] \\
&= P[Y_{ij}[t] = 1, Y_{ij'}[t] = 1] - \mathbb{E}[Y_{ij}[t]]\mathbb{E}[Y_{ij'}[t]] \\
&= P[Y_{ij}[t] = 1] \cdot P[Y_{ij'}[t] = 1|Y_{ij}[t] = 1] - \mathbb{E}[Y_{ij}[t]]\mathbb{E}[Y_{ij'}[t]] \\
&= \frac{w[t]}{|\wedge|} \cdot \frac{n_{jj'}}{w[t]} - \frac{w[t]^2}{|\wedge|^2} = \frac{n_{jj'}}{|\wedge|} - \frac{w[t]^2}{|\wedge|^2},
\end{aligned}$$
(19)

where $n_{jj'}$ is the number of hyperwedges that the *j*-th and *j'*-th instances share. However, since hyperwedges are sampled independently (specifically, uniformly at random with replacement), if $i \neq i'$, then $Cov(Y_{ij}[t], Y_{i'j'}[t]) = 0$. This observation, Eq. (14), Eq. (18), and Eq. (19) imply

$$\begin{split} & \mathbb{V}\mathrm{ar}[\hat{m}[t]] = \mathbb{V}\mathrm{ar}[\sum_{i=1}^{r} \sum_{j=1}^{M[t]} Y_{ij}[t]] \\ &= \sum_{i=1}^{r} \sum_{j=1}^{M[t]} \mathbb{V}\mathrm{ar}[Y_{ij}[t]] + \sum_{i=1}^{r} \sum_{j \neq j'} \mathbb{C}\mathrm{ov}(Y_{ij}[t], Y_{ij'}[t]) \\ &= r \cdot M[t] \cdot \left(\frac{w[t]}{|\wedge|} - \frac{w[t]^2}{|\wedge|^2}\right) + r \sum_{n=0}^{1} q_n[t] \cdot \left(\frac{n}{|\wedge|} - \frac{w[t]^2}{|\wedge|^2}\right), \end{split}$$

where $q_n[t]$ is the number of pairs of h-motif t's instances that share n hyperwedges. This and Eq. (16) imply Eq. (7) and Eq. (8).

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