A Graph Entropy Measure From Urelement to Higher-Order Graphlets for Network Analysis

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Abstract—Graph entropy measures have recently gained wide attention for identifying and discriminating various networks in biology, society, transportation, etc. However, existing methods cannot sufficiently explore the structural contents by merely considering the elementary invariants of a graph, ignoring the underlying patterns in higher-order features. In this paper, we propose a general entropy-based graph representation framework (GREET) based on four pertinent properties of graph topology from urelement to higher-order statistics. Specifically, we introduce an unbiased graphlet estimation strategy for obtaining both urelement and higher-order statistics. Additionally, we define a novel family of information functions based on hierarchical topological features to compute the graph entropy, then construct a graph information entropy (GIE) vector using the obtained local and global structural statistics to facilitate downstream tasks. Furthermore, there are some advantages that our GREET exhibits over other methods: (a) high accuracy with <1% relative error; (b) scalable for even larger vertex graphlets; (c) efficient calculation procedure with feasible speedup. Extensive experiments show that GREET exhibits superior performance on graph classification and clustering tasks, achieving remarkable improvements compared to several baselines. Altogether these findings pave the way for a wide range of applications of graphlet-based entropy as a complexity metric in graph analysis.

Index Terms—Graph entropy, induced subgraphs, higher-order graphlets, graphlet estimation, graph characterization.

I. INTRODUCTION

There are ubiquitous graph structures in various real-world complex systems, which call for trustworthy and effective graph characterization paradigms for more accurate and ultimately more useful representations. During the past decades, dozens of graph representation methods have been proposed for many networks, including communication networks [1], [2], social networks [3], [4], and biological networks [5], [6], etc. Generally, representation learning for networks is widely considered as a promising yet more challenging task, which requires the advancement of many techniques. One important issue in network characterization is to measure the complexity of these networks [7]–[9], by summarizing the underlying graph structure such as the micro-macro structure, community structure, core-periphery structure, etc.

To explore the inherent structural complexity of graphs, many entropy-based methods are presented [10]–[12]. Historically, the entropy measure originates from information theory and is used to describe the chaos of a system. Built upon the Shannon entropy, the graph entropy is usually associated with features defined on a finite graph such as the probability distribution of vertices [13], [14], edge automorphism group [15], and degree sequence of the subgraph [16], etc. However, the entropy of a graph defined by those elementary properties may encounter severe difficulties in distinguishing the non-isomorphic graphs with similar structural roles and functions. For example, it is confusing to compare the compound networks, which contain different groups with homologous benzene rings [17]. In this case, the graph entropy based on shallow features merely stands for the structural similarity, which cannot capture the underlying patterns and does not consider higher-order organizations.

Graphlets or induced subgraphs [18], [19], as basic building blocks, represent the mesoscale structure of a network, which play an important role in structural measurement, function interpretation, and a wide range of network analysis applications. It has been proved that graphlets are very effective in characterizing networks [20]–[22]. For example, the graphlet kernel [23] (defined as the dot product of two vectors of normalized graphlet counts) and the euclidean distance between graphlet frequency distribution (GFD) vectors [24], are used proverbially for many network analysis tasks. Therefore, a question can be raised naturally that “what about defining graph entropy measures by such structures?”, which has not been well studied in the literature. Interestingly, as a special kind of subgraph, the main obstacle in practical applications comes from the heavy computational budget when counting the graphlets. As shown in Table I, the number of graphlets increases exponentially with the number of vertices, which makes conducting downstream tasks highly inefficient. Furthermore, the existing algorithms [24]–[27] such as the exact counting methods, are severely limited to the network size. Hence, it is necessary to find an approximate method with high accuracy and scalability that can be used for calculating graph entropy efficiently.

In this paper, we present GREET [1], a network representation

1GREET is an anagram of the bold letters in nEtwork characTerization with GRaph Entropy.
framework based on graph entropy measure. The motivation of this work is to construct a feature vector, called graph information entropy (GIE), which represents the structural complexity of a graph and can be used for distinguishing graphs. In particular, this paper proposes unbiased graphlet estimators for deriving both urelement and higher-order graphlet statistics. The graphlet estimators provide fast and accurate approximations compared to the existing exact counting algorithms. Concretely, we design an edge-centric neighborhood with predefined settings, where tree and cyclic graphs are treated as the initial evolutionary state, indicating that the subsequent search process of the higher-order graphlet is based on these basic structures and makes the exploration process more efficient. Tree and cyclic graphs are treated as the evolutionary factors, which make the exploration process of graphlets more efficient. With the above designs, the proposed GREET achieves several orders of magnitude faster than the traditional iteration methods.

Inspired by the entropy theory in [28], we propose a novel family of information functionals based on the urelement and higher-order graphlet statistics (e.g., the frequency of $k$-vertex graphlets in an edge-centric neighborhood), which is then used to compute the graph entropy in the transformed space. It is noted that GREET only considers the graphlets that possess up to four vertices for performance and computation trade-offs. It can be easily inferred from Table I that the number of graphlets reaches 21 and 112 with five and six vertices, respectively, which are too rare for real-world networks and are too vague for characterizing a graph [16], [19], [20], [29]. Moreover, we justify the motivation of jointly considering urelement and higher-order features from the following aspects. First, it is obvious that only considering a node, edge, or its reachable nodes at a fixed distance with little flexibility changeability provides less structural information than higher-order closures. Second, taking both urelement and higher-order graphlets properties into account can obtain richer representation of the structural features of a graph.

In summary, this paper makes the following contributions:

- We propose a general network characterization framework GREET. A general network characterization framework GREET is proposed for graph comparison, which provides a novel graph entropy-based measurement for graph comparison. This framework is shown to be accurate, efficient, comprehensive, and scalable for various graph analysis tasks.

- Within the GREET framework, we develop unbiased estimators with fast and accurate counting strategies for estimating both urelement and higher-order statistics. We propose unbiased estimators for GREET framework, which provides fast and accurate counting strategies for both urelement and higher-order statistics. Experimental results on various networks show that our proposed algorithm method reduces the computational time by several orders of magnitude and achieves less than 1% relative error for nearly all graphlets.

- Motivated by Shannon entropy theory, we define two novel local and global information functionals based on the urelement and higher-order statistics, respectively. The resulting graph information entropy vector contains comprehensive complexity features both local and global topological properties of the graph while capturing the underlying structural information.

- Extensive experiments are conducted over twenty real-world networks from six domains to evaluate the proposed GREET method in terms of graph classification and graph clustering tasks. The experimental results demonstrate that GREET significantly outperforms the baselines in terms of classification accuracy and show that our proposed GIE can be used as a discriminative metric to greatly improve the graph clustering performance.

The remainder of this paper is organized as follows. Section II introduces some necessary definitions and concepts that will be used in this paper and explains the proposed framework. Section III proposes a novel family of graph characterization based on the graph entropy theory. Section IV presents extensive experimental results on several graph analysis tasks over twenty networks. Section V concludes this paper with discussions and future works.

### II. Preliminaries

In this section, we introduce some definitions and necessary notations that will be used in this paper. Besides, we formally explain the goal of this paper to obtain accurate representations of networks with a graph entropy-based measure.

Let $G(V, E)$ be a simple undirected graph with a finite non-empty set of vertices $V = \{v_1, v_2, \ldots, v_N\}$ and a finite set of edges $E = \{e_1, e_2, \ldots, e_M\}$. The existence of a edge between any two target vertices are determined by the neighborhoods centered on them. Hence, given a vertex $v_i \in V$, let $\Gamma^h(v_i) = \{v \in V \mid d(v, v_i) \leq h\}$ be the set of vertices $h$-hop adjacent to $v_i$ in $G$, where $d(v, v_i)$ is the distance between node $v$ and $v_i$ in hops. Similarly, given two vertices $v_i, v_j \in V$, let $\Gamma^h(v_i, v_j)$ denotes the $h$-hop neighborhood around them defined as

$$\Gamma^h(v_i, v_j) = \Gamma^h(v_i) \cup \Gamma^h(v_j) \setminus \{v_i, v_j\}$$

### Table I

**Distinct Notations and Properties for 2-, 3- and 4-Vertex Graphlets.** Among them, $\Delta$ and $d$ denote the max and average degree, respectively; $\rho$ denotes the density; $r$ is the assortativity coefficient; Tree and Cyclic hold true if the graphlet satisfies the requirement.

<table>
<thead>
<tr>
<th>Graphlet</th>
<th>Notation</th>
<th>$\Delta$</th>
<th>$d$</th>
<th>$\rho$</th>
<th>$r$</th>
<th>Tree</th>
<th>Cyclic</th>
</tr>
</thead>
<tbody>
<tr>
<td>$g_0$</td>
<td>0</td>
<td>1.0</td>
<td>1.00</td>
<td>1.00</td>
<td>✓</td>
<td>✓</td>
<td>x</td>
</tr>
<tr>
<td>$g_1$</td>
<td>1</td>
<td>1.33</td>
<td>0.67</td>
<td>-1.00</td>
<td>✓</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>$g_2$</td>
<td>2</td>
<td>2.00</td>
<td>1.00</td>
<td>1.00</td>
<td>✓</td>
<td>✓</td>
<td>x</td>
</tr>
<tr>
<td>$g_3$</td>
<td>2</td>
<td>1.5</td>
<td>0.50</td>
<td>-0.50</td>
<td>✓</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>$g_4$</td>
<td>3</td>
<td>1.5</td>
<td>0.50</td>
<td>-1.00</td>
<td>✓</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>$g_5$</td>
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<td>2.0</td>
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<td>1.00</td>
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<td>✓</td>
</tr>
<tr>
<td>$g_6$</td>
<td>3</td>
<td>2.0</td>
<td>0.67</td>
<td>-0.71</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>$g_7$</td>
<td>3</td>
<td>2.5</td>
<td>0.83</td>
<td>-0.66</td>
<td>x</td>
<td>✓</td>
<td>✓</td>
</tr>
<tr>
<td>$g_8$</td>
<td>3</td>
<td>3.0</td>
<td>1.00</td>
<td>1.00</td>
<td>✓</td>
<td>✓</td>
<td>✓</td>
</tr>
</tbody>
</table>
Four Properties of Graphlet Topology in Greet From the Perspective of Hierarchy and Dimension

<table>
<thead>
<tr>
<th>Hierarchy</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>Urelement</td>
<td>Single Real-Value, Distribution in local closures</td>
</tr>
<tr>
<td>Higher-Order</td>
<td>Global graphlet counting, GFD of a node/edge</td>
</tr>
<tr>
<td>Norelement</td>
<td>GFD of graphlets in G</td>
</tr>
</tbody>
</table>

For simplicity, the local neighborhood consists of the set of vertices adjacent to \( v_1 \) or \( v_2 \) and all edges between that set are denoted as \( \Gamma \). Moreover, the degree of a vertex \( v \) is denoted as \( d_v = |\Gamma^1 (v)| \) and \( \Delta (G) \) denotes the maximum vertex degree.

**Definition 1 (Graphlet).** A graphlet of \( G \), \( g_i = (V', E') \), is a connected induced subgraph of \( G \) if \( V' \subseteq V \) and \( E' \subseteq E \) with constraints that \( \{ e = (u, v) \mid u, v \in V', e \in E, e \notin E' \} = \emptyset \). In other words, graphlet is a subset of the vertices in graph \( G \) as well as all edges whose endpoints are both in this subset.

In this paper, we define a graphlet with \( k \) vertices, as \( g^{(k)} \) or \( k \)-graphlet and \( g = g^{(1)} \cup \cdots \cup g^{(k)} \). Besides, we also follow the definition in [24] that a \( k \)-graphlet is called a tree graphlet if it has \( k - 1 \) edges and the rest are named as cyclic graphlet. Table II reports some graphlet notations and important attributes.

**Definition 2 (Graphlet Frequency Distribution).** Let \( G \) be a graph, the value \( f_i^G = (X_i / \sum_i X_i) \) for \( i = 1, \ldots, |g| \) is called GFD, where \( X_i \) is the frequency of graphlet \( g_i \). The \( f^G = [\cdots f_i^G \cdots] \) is the GFD in vector form.

**Definition 3 (Shannon Entropy [30]).** Let \( X \) be a discrete random variable. The Shannon entropy of \( X \) is defined as

\[
I_X = -\sum_x p(x) \log p(x)
\]

\[
I_X = -\sum_{x \in X} p(x) \log (p(x)),
\]

where \( p(x) \) denotes the probability mass function that \( X \) is in the state \( x \) where \( p(x) \) is the probability distribution of \( X \).

**A. Graph Entropy and Information Functional**

Combining the Shannon entropy [30] with graph theory [31], Dehmer et al. [28] proposed a new complexity measure that is graph entropy. One of the salient features for this graph entropy is that we can capture the structural content through parameterized representation.

**Definition 4 (Dehmer [28]).** Given an undirected simple graph \( G \), for a vertex \( v_i \in V \), its local information functional is defined as

\[
f(v_i) = \alpha S_1(v_i, G) + \beta_2 S_2(v_i, G) + \cdots + \beta_p S_p(v_i, G)
\]

where \( \alpha \) is arbitrary real positive coefficient as well as \( \beta_k \) for \( k = 1, 2, \ldots, p \). \( S_p(v_i, G) \) denotes the number of vertices in \( p \)-sphere, which acts as the set \( \{ v \in V \mid d(v_i, v) = \rho, \rho \geq 1 \} \).

The local information functional exploits the intrinsic graph topology. Consequently, the vertex probability distribution based on information functional can be written as

\[
p(v_i) = \frac{f(v_i)}{\sum_{v_j \in V} f(v_j)}
\]

Subsequently, the graph entropy can be calculated in the form of Shannon entropy once a frequency distribution of the vertex set is obtained, which motivates us to associate the frequency of different structures with graph characterization.

**B. Problem Formulation**

The objective of this study is to explore a variety of graphlet statistics so as to construct a more discriminative feature vector for designing a practical graph representation learning framework. Inspired by [32], we mainly focus on two pairs of statistics with hierarchical and dimensional differences: urelement versus higher-order graphlets and single real-value versus distribution. Here, we provide an intuitive explanation for four properties of graphlet topology that are keys for learning powerful graph representations.

- Two notions of urelement are defined for local properties. The first, single real-value urelement statistics, refers to the elementary structural features, e.g., the degree power of vertices, the counts of triangle graphlet containing a certain node or edge in the local neighborhood \( \Gamma_c \). The second, urelement distribution, measures an individual graph element (an arbitrary node or edge) through GFD.
- There are two further properties related to global structural information. Higher-order single real-value statistics can be defined as the total number of arbitrary graphlets in graph \( G \). As the dimensional expansion, higher-order distribution indicates the overall graphlet frequency distribution (GFD) of \( G \).

The proposed framework gives rise to graphlet feature exploration methods that are effective and efficient for various network applications. Recent approaches are limited to unilaterial statistics [16], [20], [24], [33], whereas this paper instead proposes a comprehensive characterization framework beyond single counts that combines multidirectional graphlet statistics with information entropies.

**III. THE PROPOSED METHOD**

In this section, we introduce a novel family of graph entropy measures (GREET) by exploring urelement and higher-order graphlet statistics. This gives rise to the graphlet-based entropy measure that serves as a basis for deriving fast and accurate graph representations which are also applicable and scalable for networks in different domains. An illustration of the GREET framework is depicted in Fig. [1] for intuition.

**A. The Urelement Statistics Estimating Method**

Given the sampled target set of edge-centric neighborhoods, we illustrate the way to calculate the estimation of all distinct graphlets containing a specific node or edge in Algorithm [1]. Specifically, the process of estimating the urelement statistics for an individual node or edge mainly consists of two parts,
denoted by \( y \) represents the approximation of the exact urelement statistics \( 0 \) to \( 8 \). Among them, all graphlets used in this paper, referred as those in tree namely the tree and cyclic graphlet enumeration. Table 1 lists all graphlets used in this paper, referred as \( g_i \) for \( i \) ranging from \( 0 \) to \( 8 \). Among them, \( g_1, g_3, \) and \( g_4 \) are tree graphlets while the remaining are cyclic graphlets. The task of urelement statistics estimation is to calculate an accurate yet fast approximation of graphlet distribution over a local neighborhood.

**Definition 5 (Urelement Estimation).** Given an undirected graph \( G = (V, E) \) and an edge-centric local neighborhood \( \Gamma_r \), the urelement estimation problem is to minimize function \( L(u_i; y_i) \), where \( u_i = [u_1^i \ u_2^i \ \cdots \ u_5^i \ u_6^i \ \cdots \ u_8^i]^T \) represents the approximation of the exact urelement statistics denoted by \( y_i \) for edge \( e_i \in E \). The element \( u_k^i \) in \( u_i \), for \( k \) from \( 1 \) to \( 8 \) corresponding to the graphlet \( g_i \) presented in Table 1.

Here, \( L1\text{-}norm \) is adopted as the loss function in Definition 5. Along the searching method proposed in [34], we commence by classifying basic substructures into tree and cyclic. First of all, we explain the searching of tree graphlet. Instead of discovering all tree graphlets explicitly, we relax the above problem through a general paradigm. Let us denote \( \Gamma \) as the target 1-hop neighborhood with respect to \( e(u, v) \in E \). We construct two sets of nodes \( N_u = \{ s \in \Gamma(u) \setminus \{ v \} | s \notin \Gamma(v) \} \) and \( N_v = \{ r \in \Gamma(v) \setminus \{ u \} | r \notin \Gamma(u) \} \) within \( \Gamma \), that complete simplest tree graphlet with node \( u \) and \( v \), respectively. For further intuition, please see Fig. 2. These defined structures are enable us to easily count the quantities of \( g_1 \). Furthermore, other tree graphlet such as \( g_3, g_4 \) or trees with more vertices can be found by the combinations of centered edge and \( N_u, v \). As for the enumeration of cyclic graphlet, we can utilize partial known spanning trees to generate cyclic graphlets (e.g., \( g_6, g_7 \) can have \( g_1, g_3, \) and \( g_4 \) as their precursor tree graphlets).

We now discuss the urelement estimation problem in detail. Let us set \( \psi(\cdot) \) as a node label function for facilitating later procedure. Thus, nodes in local neighborhoods are labeled as \( \theta_1, \theta_2, \) and \( \theta_3 \). Specifically, the neighbors \( \Gamma(u) \) of \( u \) are marked as \( \theta_1 \). Likewise, the neighbors \( \Gamma(v) \) of \( v \) and the nodes in \( D_e \) are labeled as \( \theta_2 \) and \( \theta_3 \), respectively. First and foremost, sets \( N_u, N_v, \) and \( D_e \) are investigated by following iterations.

- **Start with an edge** \( e = (u, v) \in E \) and let \( N_u, N_v, \) and \( D_e = \{ \} \).
- **for each node** \( s \in \Gamma(u) \), if \( s \neq v \) then update \( N_u \leftarrow N_u \cup \{ s \} \) and set \( \psi(s) = \theta_1 \).
- **for each node** \( s \in \Gamma(v) \) – \( u \), if \( \psi(s) = \theta_1 \) then update \( D_e \leftarrow D_e \cup \{ s \} \), \( N_u \leftarrow N_u - \{ s \} \) and set \( \psi(s) = \theta_3 \); else update \( N_v \leftarrow N_v \cup \{ s \} \) and set \( \psi(s) = \theta_2 \).
- **Repeat the steps** until all nodes in \( \Gamma \) are investigated.

As shown in Algorithm 1, for simple 3-vertex graphlet \( g_1 \) and \( g_2 \), their estimation can be obtained directly via Lines 17–18 (as observed in [35]). Then, we investigate each \( s \in N_v \) and select a vertex \( r \in \Gamma(s) \) with predefined probability distribution \( P \). Apparently, \( g_5 \), the 4-vertex cyclic graphlet can be checked by judging the type of vertex \( r \) and the intermediate variables.
Algorithm 1 Estimation of Urelement Statistics

**Input:** An edge-centric neighborhood $\Gamma_e$ and a sampling factor $p$

1. for each $s \in N_u$ do
2.   for $k = 1$ to $|[d_s]_p|$ do
3.     Sample a vertex $r \in \Gamma(s)$ with a given distribution $P$
4.     if $\psi(r) = \theta_1$ then update $u_5 = u_5 + (d_s/|[d_s]_p|)$ \(\triangleright g_5\)
5.     if $\psi(r) = \theta_2$ then update $u_6 = u_6 + (d_s/|[d_s]_p|)$ \(\triangleright g_6\)
6.     Reset $\psi(s) = 0$
7. for each $s \in N_v$ do
8.   for $k = 1$ to $|[d_s]_p|$ do
9.     Sample a vertex $r \in \Gamma(s)$ with a given distribution $P$
10. if $\psi(r) = \theta_1$ then update $u_6 = u_6 + (d_s/|[d_s]_p|)$ \(\triangleright g_6\)
11. Reset $\psi(s) = 0$
12. for each $s \in D_e$ do
13.   for $k = 1$ to $|[d_s]_p|$ do
14.     Sample a vertex $r \in \Gamma(s)$ with a given distribution $P$
15. if $\psi(r) = \theta_1$ then update $u_8 = u_8 + (d_s/|[d_s]_p|)$ \(\triangleright g_8\)
16. Reset $\psi(s) = 0$
17.   for each $s \in N_u$ do
18.     $u_1 = (d_u + d_v - 2) - 2|D_e|$ \(\triangleright g_1\)
19.     $u_2 = |D_e|$ \(\triangleright g_2\)
20.     $u_3 = |N_u| \cdot |N_v| - u_5$ \(\triangleright g_3\)
21.     $u_4 = C^m_{|N_u|} \cdot C^m_{|N_v|} - u_6$ \(\triangleright g_4\)
22. end return, where $u_i$ is the estimate of graphlet $g_i$ in $\Gamma_e$.

$\theta_1$, as an indication that whether there exists potential edges between nodes in sets $N_u$ and $N_v$. Lines 5, 7–11 also show the detection of $g_6$ under the similar condition as $g_5$. In addition, the 4-vertex fully connected cyclic graphlet $g_4$ are estimated by searching area $D_e$, in which a node participates a triangle directly. Ultimately, the rest of graphlets are estimated in $O(1)$ time using previous knowledge (Lines 19–21). Among them, the 4-vertex lines $g_8$ are calculated by subtracting those completing a cyclic, while graphlets $g_4$ and $g_7$ are estimated leveraging the combination number formula, where $C^m_n = n!/(m!(n-m)!)$.

**Complexity Analysis:** The strategy we adopted enables us to estimate the urelement statistics efficiently, which utilizes the obtained knowledge in each step adequately. By dividing graphlet into two typical structures, namely the tree graphlet and the cyclic graphlet, we are able to extrapolate other more complex graphlets. Furthermore, compared to the existing methods [24], [25], [29], we specify three key sets $N_u$, $N_v$, and $D_e$ that makes it possible to count $k$-vertex graphlets without unnecessary computation. Finally, to calculate the urelement statistics from a given edge, the computational complexity is $O(\Delta(|N_u| + |N_v| + |D_e|))$, where $\Delta$ denote the maximum degree of vertex within $N_u$, $N_v$, and $D_e$. It is evident that most of the computational budget comes from the searching process of neighbors in the above sets. To mitigate this problem, we predefine sampling factor $p$ (Lines 3, 9, and 14), which ensures the acquisition of important network structure while leading to an acceptable time cost.

**B. The Higher-Order Statistics Estimating Method**

This section discusses graphlet estimation in the context of the entire graph. Note that, we retain some necessary notations and illustrations from Section III-A for better understanding. It is necessary to investigate the difference between urelement and higher-order graphlet estimation strategies. Obviously, there exist more diverse connection patterns among the whole graph than local subgraphs, resulting in unavoidable counting errors. On account of this, we adopt the Horvitz-Thompson estimator [36] to obtain unbiased estimates. The iterative process is shown in Algorithm 2. First, for each sampled edge $e \in E_s$, we build neighborhoods $N_u$, $N_v$, and $D_e$, as it was done in Section III-A. The quantity of $g_1$, $g_2$, $g_4$, $g_6$, and $g_7$ are derived in $O(1)$ time utilizing knowledge from the centered edge and its completed tree and cyclic structures with sets $N_u$, $N_v$, and $D_e$ (refer to Lines 4–7, and 9–10 in Algorithm 2 where $\oplus$ denotes the addition assignment operator). Besides, the $g_5$ and $g_8$ are computed through Algorithm 3 and using information from the $(k-1)$-vertex tree and cyclic graphlets. Here, we use $H_i$ for $i$ from 1–8 to denote the graph component counts in graph $G$ and sampling probability $p_i$ is defined as $p_i = |E_s|/|E|$, where $|E_s|$ and $|E|$ are the number of sampled edges and total edges in graph $G$, respectively. Moreover, let the reciprocal of $p$ be $z_i = 1/p_i$, which is then used to correct the counting errors.

Intuitively, the sampling bias can be easily associated with the edge role in each graphlet. As shown in Fig. 3, we highlight all qualified edges in red color and list a table in the bottom-right corner, which concludes the number of suitable edges per each graphlet.

Algorithm 2 Estimation of Higher-Order Statistics

**Input:** A graph $G(V, E)$ with sampled edge set $E_s$

1. for each $e = (u, v) \in E_s$ do
2.   Set $D_e$, $N_u$, and $N_v = \emptyset$
3. Construct local neighborhoods as in Alg. 1
4. $H_1 \oplus H_5(e) = |N_u| + |N_v|$  
5. $H_2 \oplus H_2(e) = |D_e|$  
6. $H_3 \oplus H_3(e) = |N_u| \cdot |N_v|$  
7. $H_4 \oplus H_4(e) = C^m_{|N_u|} + C^m_{|N_v|}$  
8. $H_5 \oplus H_5(e) = S_4$-Cyc($\psi$, $N_u$)  
9. $H_6 \oplus H_6(e) = (|N_u| + |N_v|) \cdot |D_e|$  
10. $H_7 \oplus H_7(e) = C^m_{|D_e|}$  
11. $H_8 \oplus H_8(e) = S_4$-Cyc($\psi$, $D_e$)  
12. return $H_i$, where $H_i$ is the count for graphlet $g_i$.  

Fig. 3. Edge connection pattern diagram: Figure shows all possible edges that satisfied the requirements for building edge-centric neighborhoods $N_u$, $N_v$, and $D_e$. Note that, all eligible edges are colored in red and highlighted. The table in the bottom-right corner provides the summarization of qualified edges in each 2-, 3-, and 4-graphlet.
triangles. Therefore, the role of each edge in \(g_8\) is exactly the same and all of them satisfy the definition of the central edge. Similarly, consider the simplest 4-cyclic \(g_9\), where each edge is equivalent. Combined with the above views and algorithms, we can deduce that each F4-cyclic \(g_6\) and S4-cyclic \(g_9\) will be counted 6 and 4 times, respectively. As a result, the correction coefficients are given as 1/6 and 1/4. Formally, the correction factor of \(g_i\) account for the edge multiplicities in \(G\) is defined as

\[
C(\psi, G) = \frac{1}{\psi}
\]

where \(\psi\) is the number of edges that qualified for the definition of the local neighborhood in graphlet \(g_i\). Afterward, the higher-order graphlet counts are estimated via the following equations:

\[
X_i = z_iC_iZ_i, \quad Z_i = \begin{cases}
H_i & i = 1, 2, 5, 6, 8 \\
H_i - H_5 & i = 3 \\
H_i - H_6 & i = 4 \\
H_i - H_8 & i = 7
\end{cases}
\]

where \(X_i\) is the estimated counts of the graphlet \(g_i\). Specifically, the calculation of graphlets \(g_5, g_6, \) and \(g_7\) are different from the others. This is due to the fact that such graphlets are structurally evolved from basic tree and cyclic graphlets.

**Error Analysis:** For a graphlet \(g_i\), assume \(Y_i(\varepsilon)\) is its ground truth in the \(G(V, E)\). In the process of estimation, we construct edge-centric neighborhood over the sampled edges of the given graph \(G\), such that an edge \(\varepsilon\) accounts for the existence of \(g_i\). Thus, the total count of \(g_i\) are obtained as \(Y_i = \sum_{\varepsilon \in E} Y_i(\varepsilon)\). The approximation counting method of \(GREET\) estimate \(Y_i\) by sampling a set of edges \(E_s \subset E\) using a certain probability \(\tau\), then

\[
X_i \geq \frac{1}{\tau} \sum_{\varepsilon \in E_s} Y_i(\varepsilon)
\]

is an estimator for \(g_i\).

**Lemma 1.** \(X_i\) is an unbiased estimator of \(Y_i\).

**Proof.**

\[
E[X_i] = E \left[ \frac{1}{\tau} \sum_{\varepsilon \in E_s} Y_i(\varepsilon) \right] = \frac{1}{\tau} \sum_{\varepsilon \in E_s} E[Y_i(\varepsilon)]
\]

Since each of the edges are sampled randomly, \(E[Y_i(\varepsilon)] = E[B_\varepsilon] \cdot Y_i(\varepsilon)\), where \(B_\varepsilon\) denotes a Bernoulli random variable indicating whether \(\varepsilon\) and its local neighborhood are selected. Plugging in Eq. \(\text{(8)}\) we obtain:

\[
E[X_i] = \frac{1}{\tau} \sum_{\varepsilon \in E} E[B_\varepsilon] \cdot Y_i(\varepsilon) = \frac{1}{\tau} \sum_{\varepsilon \in E} \tau \cdot Y_i(\varepsilon) = Y_i
\]

Hence, the lemma is proved. \(\square\)

Moreover, the mean squared error (MSE) of \(X_i\) is obtained as \(E[(X_i - Y_i)^2]\). Since, \(E[X_i] = Y_i\) and we have

\[
\text{MSE}(X_i) = \frac{\text{Variance} + \text{Bias}}{\text{Bias}}
\]

where the first term on the right side of the equation is variance and the second term is the bias generated by the estimator \(X_i\).

As a result, since \(X_i\) is an unbiased estimator, \(\text{MSE}(X_i) = \mathbb{E}[(X_i - E[X_i])^2] = 0\).

**Algorithm 3 Simplest 4-Cyclic Counting**

1. **procedure** S4-CYCLIC(\(\psi, N_s\))
2. Set variable \(C_s = 0\)
3. **for** each \(s \in N_s\) **do**
4. **for** each \(r \in \Gamma(s)\) **do**
5. if \(\psi(r) = \theta_1\) then set \(C_s \oplus 1\)
6. **end do**
7. **end for**
8. **end for**
9. **return** \(C_s\)

**Algorithm 4 Fully-Connected 4-Cyclic Counting**

1. **procedure** F4-CYCLIC(\(\psi, D_s\))
2. Set variable \(C_f = 0\)
3. **for** each \(s \in D_s\) **do**
4. **for** each \(r \in \Gamma(s)\) **do**
5. if \(\psi(r) = \theta_2\) then set \(C_f \oplus 1\)
6. **end do**
7. **end for**
8. **end for**
9. **return** \(C_f\)

**C. Quantifying Structural Information with Entropy**

Given the hierarchical graphlet statistics, a straightforward way is to directly transform these counts into heuristic features, which turns out to be suboptimal in \(\text{\cite{37}}\), probably due to the lack of generality. To address this, we present two novel information functionals based on a fixed size of induced subgraphs, which can be utilized to estimate the entire graph entropy. Then, such graph entropies are combined with other topological information content metrics to construct discriminative and general graph representations that can be computed efficiently.

Different from Dehmer’s work \(\text{\cite{28}}\), we cast sight on defining the probability distribution of edges for a graph. In this paper, we introduce an edge-centric neighborhood \(\Gamma_e\) with abundant properties, which allows us to define graph entropy based on the obtained urelement and higher-order graphlet statistics (Table \(\text{\cite{11}}\). As mentioned in \(\text{\cite{28}}\), such graph entropies can capture the underlying structural information of \(G\) effectively.

**Definition 6 (Edge Probability Distribution).** Let \(G = (V, E)\) with iterable edge labels. For an edge \(e_i \in E\), we define

\[
p(e_i) := \frac{f(e_i)}{\sum_{j=1}^{N(E)} f(e_j)}
\]
where \( f(\cdot) \) represents an information functional, which satisfied the equation \( p(e_1) + p(e_2) + \cdots + p(e_{\mid E\mid}) = 1 \).

**Definition 7 (Graph Entropy).** Given a undirected graph \( G = (V,E) \) and let \( f \) be an arbitrary information functional. We define the entropy of \( G \) by

\[
I_f(G) = -\sum_{i=1}^{\mid E\mid} \frac{f(e_i)}{\sum_{j=1}^{\mid E\mid} f(e_j)} \log \left( \frac{f(e_i)}{\sum_{j=1}^{\mid E\mid} f(e_j)} \right)
\]

**Definition 8 (Local Information Functional).** Given a simple undirected graph \( G \), the local information functional for an edge \( e_i \in E \) is given as

\[
f^U(e_i) := e^{\alpha_1\mid u_1(e_i,G) + \alpha_2\mid u_2(e_i,G) + \cdots + \alpha_k\mid u_k(e_i,G)}
\]

where \( \alpha_k \) is the real positive coefficient. \( \mid u_k(e_i,G) \) indicates the estimated uelement statistics of neighborhood \( \Gamma e_i \) regarding \( G \).

**Definition 9 (Global Information Functional).** For a given graph \( G = (V,E) \), let \( h_j(G) \) be the number of graphlet \( g_j \). We define the global information functional by

\[
f^H(G) := h_j(G)
\]

where \( j \) is the ordinal number of graphlet.

Apparently, according to the above definition, we can obtain \( h_j(G) \) directly from the estimation of higher-order graphlets. Let \( \theta(G) = \sum_{j=1}^{T} h_j(G) \) be the total number of graphlets in \( G \), \( T \) is the number of types of graphlets. The obtained graph entropy \( I_f^H \) is stated as

\[
I_f^H(G) = -\sum_{j=1}^{T} \frac{f^H(G)}{\theta(G)} \log \left( \frac{f^H(G)}{\theta(G)} \right)
\]

Similarly, the graph entropy \( I_f^U \) is stated as

\[
I_f^U(G) = -\sum_{i=1}^{\mid E\mid} \frac{f^U(e_i)}{\sum_{j=1}^{\mid E\mid} f^U(e_j)} \log \left( \frac{f^U(e_i)}{\sum_{j=1}^{\mid E\mid} f^U(e_j)} \right)
\]

In particular, the general idea in computing the information functional \( f^U(e_i) \) and \( f^H(G) \) is that we build a bridge between the simple counts of graphlets and the measurement of graphs from the perspective of micro and macro. One prominent advantage of this method is that it quantifies the structural information of a graph with meaningful complexity measurement.

**Numerical Analysis:** We numerically investigate the entropies of the example graphs of Fig. 4 by using the proposed information functional \( f^U(e_i) \) and \( f^H(G) \). Based on the obtained estimation results of uelement and higher-order graphlet statistics, we are able to explore the discernibility of the resulting graph entropies. For \( G_1 \), by applying the Algorithm [4] we obtain:

\[
f^U(e_2) = \frac{e^{\alpha_1+\alpha_2+\alpha_4+\alpha_5}}{e^{2\alpha_1+\alpha_4}}
\]

\[
f^U(e_3) = \frac{e^{\alpha_3+\alpha_5}}{e^{2\alpha_1}}
\]

\[
f^U(e_1) = e^{2\alpha_1}
\]

Here, we set \( \alpha_1 = \alpha_2 = \cdots = \alpha_k = 1 \) and plug \( f^U(e_i) \) into Eq (16). Thus, the structural content of \( G_1 \) becomes to

\[
I_f^U(G_1) = -\frac{e^2}{2e^2 + 2e^2 + e^3} \log \left( \frac{e^2}{2e^2 + 2e^2 + e^3} \right)
\]

To compute the entropy of \( G_1 \) regarding \( f^H \), we directly apply Definition 9 to the Eq. (13) and obtain:

\[
I_f^H(G_1) = -\frac{2}{3} \log \left( \frac{1}{3} + \frac{1}{3} \log \frac{1}{6} \right)
\]

By applying the same steps as stated above, the calculation for the structural information of \( I_f^U(G_2) \) and \( I_f^H(G_2) \) is the same. Hence,

\[
I_f^U(G_2) = -\frac{1}{2} \left( \frac{e^3}{4e^3 + e^{10}} + \frac{e^{10}}{4e^3 + e^{10}} \right)
\]

\[
I_f^H(G_2) = -\frac{1}{2} \left( \frac{1}{2} \log \frac{1}{2} + \frac{1}{3} \log \frac{1}{3} + \frac{1}{6} \log \frac{1}{6} \right)
\]

Obviously, the computation of \( I_f^U(G) \) is able to generalize to more complicated structures. As mentioned earlier, we mainly consider 3- and 4-graphlets due to the computational cost. To guarantee the independence and the discrimination of features, we combine some variants of \( I_f^U \) and \( I_f^H \) with other classical graph entropy metrics to construct the graph information entropy (GIE) vector for a richer graph representation. Specifically, we add the graph entropy \( I_\alpha \) and \( I_d \) proposed in \([38\), \([39\], which are defined by the vertex orbits and the degree sequence of all vertices in \( G \), respectively. Motivation of this setting is straightforward. Firstly, the metrics \( I_\alpha \) and \( I_d \) are nearly the simplest version of the graph entropy, which can be utilized to improve the discrimination ability in distinguishing networks with significant structural differences. Secondly, incorporating
various graph entropy can receive better generalization capability. As a result, the complete form of the feature vector is \( \vec{v}_{GIE} = [I_{f_1}^v, I_{f_2}^v, I_{f_2}^v + I_{f_3}^v, |I_{f_1}^v||I_{f_2}^v|, I_0, I_2] \), which measures both local and global structure information of a graph and can be fed into a neural network or machine learning model for downstream tasks.

IV. EXPERIMENTS

In this section, we conduct extensive experiments to evaluate the performance of GREET on over twenty networks from six domains with different structural properties. All datasets are obtained from the Network Repository and an open source dataset website\(^4\). To make a fair comparison, our experiments are performed on a Windows (64-bit) PC with a Quad-Core Intel i5-9300HF CPU 2.4GHz processor, 16GB RAM, and NVIDIA GeForce GTX 1660Ti 6G GPU.

A. Performance on the Higher-Order Graphlet Estimation

The first class of experiments investigates the performance of GREET on higher-order graphlet estimation problems. We select twenty undirected graphs as testbeds including biological, social, interaction, collaboration, email, and economic networks. Table III reports the statistical information of each network. Here, the state-of-the-art approach PGD is utilized to compute the exact graphlet counts for comparison. In our experiments, we define \( \hat{X}_i - X_i \) as the relative error of \( X_i \), \( 1 \leq i \leq 8 \), where \( \hat{X}_i \) denotes the unbiased estimator of the genuine statistic \( X_i \). For better performance, the indicator is expected to be as small as possible. Note that all estimated values are calculated over 100 independent runs.

1) Estimating the Graphlet Statistics: We first test GREET for estimating the frequency of graphlets with size \( k = 3 \) and \( k = 4 \). Table IV lists the GFD results for a variety of real-world networks at the sampling factor of 0.1. It can be observed that tree graphlets \( g_3 \) and \( g_4 \) make up the majority of graphlets in most networks, while the proportion of cyclic graphlets \( g_2, g_5, \) and \( g_6 \) remain at the bottom on most graphs. Such results enable us to better analyze the network patterns and structural information. Besides, the L1-norm between exact counts and the estimated results are given to illustrate the high accuracy of the estimator among all graphs and graphlets.

2) Sampling Factor versus Counting Error: To fully evaluate our methods, we further explore the effect of the sampling probability on counting error. Fig. 5 reports the relative errors of GREET with sampling factor \( p = 1\%, 10\%, 100\% \). We can observe that the counting errors are proportional to \( 1/p \), which is consistent with the analysis in Section IV-C. Besides, no significant differences are found between the estimated and the exact counts in all cases. For most graphs, the counting errors of the graphlets are lower than 0.01 when \( p = 1\% \), except for those graphlets with relatively small counts. The overall trend of the results indicates that graphlets with large proportions exhibit less error than those with small proportions.

3) Speed-Up Comparison with Previous Work: In addition, we also study the computational time of GREET on eight typical networks from six domains that are shown in Table V. Three existing graphlet counting methods, including brute force \(^5\), GUFSE \(^5\), and GRAFT \(^3\), are used for comparison. However, as the graph grows larger, it is difficult to obtain accurate counting for GUFSE and GRAFT. Thus, we only report the time cost until the relative error reaches below 0.01. For large graphs, traditional brute force is clearly not suitable due to its high computational costs. Thesyphens “—” in Table V means that there is out of memory and the calculation cannot be accomplished within 3 hours. Take the large graph “ca-AstroPh” as an example, which has nearly 200k edges and is not able to be completed in a short period of time by brute force. GUFSE takes over 1 minute to compute and GRAFT returns in 18 seconds. Strikingly, our proposed GREET only takes less than 2 seconds to return the results. Benefitting from the proposed sampling strategy, for other graphs, GREET further reduces the computational time to less than 1 second. In summary, our approach is about 2 to 3 orders of magnitude faster than the traditional iteration methods, GUFSE, and GRAFT, which makes GREET a better option among various estimation methods and thus leads to higher efficiency in other tasks.

B. Comparison with Existing Works on Graph Classification

In this experiment, we evaluate the performance of GREET on graph classification tasks using eight datasets from bioinformatics and social networks. Those are PROTEINS, MUTAG, ENZYMES, COX2, IMDB-B, IMDB-MULTI, PTC-FR, and REDDIT-B datasets. Several state-of-the-art methods are used as baselines including:

- **Graph kernel-based methods**: Weisfeiler-Lehman kernels (WL) \(^4\) serves as one of the most prominent graph kernel methods for graph representation learning, which maps the...
TABLE IV
GFD ESTIMATES OF NINE GRAPHLETS FOR VARIOUS REAL-WORLD NETWORKS. ALL GFD ESTIMATES HAVE LESS THAN $10^{-4}$ ARE UNDERLINED AND THE LARGEST PROPORTION OF GRAPHLET ARE HIGHLIGHTED.

<table>
<thead>
<tr>
<th>Graph</th>
<th>GFD Estimate</th>
<th>L1-norm</th>
</tr>
</thead>
<tbody>
<tr>
<td>bio-CE-LC</td>
<td>0.0369</td>
<td>0.0005</td>
</tr>
<tr>
<td>bio-HS-HT</td>
<td>0.0213</td>
<td>0.0033</td>
</tr>
<tr>
<td>bio-dmela</td>
<td>0.0266</td>
<td>0.0001</td>
</tr>
<tr>
<td>bio-yeast</td>
<td>0.0965</td>
<td>0.0018</td>
</tr>
<tr>
<td>bio-celegans</td>
<td>0.0179</td>
<td>0.0008</td>
</tr>
<tr>
<td>soc-pg-tvshow</td>
<td>0.0277</td>
<td>0.0133</td>
</tr>
<tr>
<td>soc-wiki-vote</td>
<td>0.0373</td>
<td>0.0018</td>
</tr>
<tr>
<td>ia-corecipient</td>
<td>0.0085</td>
<td>0.0027</td>
</tr>
<tr>
<td>ia-fb-messages</td>
<td>0.0260</td>
<td>0.0004</td>
</tr>
<tr>
<td>ia-reality</td>
<td>0.0179</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>ca-GrQc</td>
<td>0.0400</td>
<td>0.0262</td>
</tr>
<tr>
<td>ca-CSphd</td>
<td>0.1359</td>
<td>0.1939</td>
</tr>
<tr>
<td>ca-AstroPh</td>
<td>0.0704</td>
<td>0.0356</td>
</tr>
<tr>
<td>email-EU</td>
<td>0.0075</td>
<td>&lt;0.0001</td>
</tr>
<tr>
<td>email-enron-only</td>
<td>0.0686</td>
<td>0.0128</td>
</tr>
<tr>
<td>email-univ</td>
<td>0.0404</td>
<td>0.0027</td>
</tr>
<tr>
<td>econ-wm1</td>
<td>0.0182</td>
<td>0.0074</td>
</tr>
<tr>
<td>econ-poli</td>
<td>0.1035</td>
<td>0.0008</td>
</tr>
<tr>
<td>econ-mahindas</td>
<td>0.0255</td>
<td>0.0003</td>
</tr>
<tr>
<td>econ-mbeaflw</td>
<td>0.0105</td>
<td>0.0013</td>
</tr>
</tbody>
</table>

Fig. 5. Relative error of estimates for graphlet $g_i$, $1 \leq i \leq 8$, given by algorithms in Section IV-C with sampling factor $p = 1\%, 10\%, 100\%$. 

This article has been accepted for publication in IEEE Transactions on Network Science and Engineering. This is the author’s version which has not been fully edited and content may change prior to final publication. Citation information: DOI 10.1109/TNSE.2022.3216803 © 2022 IEEE. Personal use is permitted, but republication/redistribution requires IEEE permission. See https://www.ieee.org/publications/rights/index.html for more information.
original graph to graph sequences with topological and label information. Shortest Path kernel [42] tackles the NP-hard problem that computes all paths and longest paths in a graph and offers a computable solution in polynomial time. Graphlet kernel [23] compare graphs by simply counting graphlets.

- **Graph neural network-based methods:** Graph convolutional networks (GCN) is a variant of convolutional neural networks that operate directly on graphs. DGCNN [47] applies a localized graph convolution model and designs a novel SortPooling layer to achieve ordered training. Graph-U-Nets [44] proposes a novel pooling strategy that employs a projection vector to measure the rank of each node. StructPool [45] models graph pooling as a node clustering problem and leverages conditional random fields (CRF) to capture the relationships among the assignments of different nodes.

- **Graph entropy-based methods:** The classical topological information content \( I_{vd} = - \sum_{i=1}^{n} d_i \log d_i \), proposed by Bonchev et al. [46], is calculated based on the degree of vertex. Dehmer [28] introduced a graph entropy measure based on the cardinalities of vertex spheres. Aziz et al. [16] defined an information functional based on the degree statistics of the graphlet, which are used to estimate the entropy of networks in a transformed space.

For this experiment, the graph entropy-based feature vector introduced in Section III-C is utilized as the input to train the classifier. Considering its simplicity and strong discriminative ability, an easily constructed three-layer fully-connected neural network is adopted as the classifier. The width of hidden layers are set to 32, 32, 16. Dropout with a rate of 0.5 is used to prevent overfitting. Besides, we adopt rectified linear unit (ReLU) and softmax function for the active function in all hidden layers and output layer, respectively. To compare the graph classification accuracies of GREET and the alternate approaches, we perform 10-fold cross-validation with 9 folds for training and the rest for testing the model, as described in [16, 23, 41, 43, 44]. We also employ the Adam optimizer [47] with a learning rate of 0.001 and a batch size of 64 for training. An early stopping mechanism is utilized for better efficiency. Specifically, for the graph entropy-based method proposed in [28, 46], we use the Euclidean distance of two metrics \( I_{vd} \) and \( I_f(G) \) between two graphs for classification. For other baselines, we use the original implementations and parameter settings released by the authors to ensure fair comparisons. All the experiments are conducted five times independently. Table VI summarizes the comparison results.

It is observed that our proposed GREET remains on the top for most datasets. Concretely, our method outperforms the previous best approach by margins of 1.94, 3.06, 3.04, 0.99, 2.33, and 4.38 percent on MUTAG, ENZYMES, COX2, IMDB-MULTI, PTC-FR, and REDDIT-B, respectively.4, 1.94, 3.06, 3.04, 2.28, 2.93, and 5.02 percent on PROTEINS, MUTAG, ENZYMES, COX2, IMDB-MULTI, PTC-FR, and REDDIT-B, respectively. The competitive performances, particularly on REDDIT-B, which has a larger number of nodes, demonstrate the effectiveness of our method in handling large graphs. It is not surprising since most graph kernel approaches are designed for capturing the shallow graph structural information, while our GREET takes both urelement statistics and higher-order graphlet features into consideration. From an overall perspective, our proposed method also performs well on other small datasets, demonstrating its generalizability. Besides, during the implementation of GNN-based methods, a severe over-fitting issue in training deep graph neural networks has been discovered to yield inferior results. It is worth mentioning that our proposed GREET gains insight into a novel measurement for graph representation, which introduces the graphlet-based entropy to address the problem of the prohibitively high training burden and thus overcome the obstacles for the subsequent tasks. Furthermore, in terms of standard deviation, the fluctuation of GREET is less than most baselines, especially compared to those GNN-based models, which also indicates the stability of our method. Moreover, we find that compared with other datasets, the experiments on ENZYMES have achieved unsatisfactory performance, i.e., the accuracy results on ENZYMES are lower than other datasets. We reckon that it is related to the design of the neural networks, which is not conducive to handling multi-classification tasks. Here, we leave it to future works.

Fig. 6 gives a further comparison of the graph classification performances on dataset PROTEINS with three different features concerned. The first uses only GFD as the input feature,
the second merely utilizes GIE as the input, and the third takes both GFD and GIE into consideration. We can observe that the concatenation feature vectors always achieve better performance than only GFD or GIE. In addition, we test the sensitivity of these variations with different training ratios. From Fig. 2, we can observe that the classification accuracy improves by 5.43, 4.13, 4.74, 4.96, and 4.51 percent with 50%, 60%, 70%, 80%, and 90% training ratio, respectively, when GIE is considered as complement term. These experiments further prove that our proposed graph entropy features can greatly promote the performance of graph classification tasks.

### C. GIE as a Property for Graph-Clustering

In this section, we also conduct experiments to demonstrate the usability of GIE for clustering graphs into their functional domains. To achieve this, we compare the performance of only GIE or GFD considered methods on twenty datasets using the mainstream agglomerative clustering technique. The Euclidean distance is utilized as the distance metric. Here, we consider a total of twenty graphs from six domains (Table III). Six graphs from the gene functional associations of biological networks, two graphs from the user social information networks, three graphs from the interaction networks, three graphs from the collaboration networks, three graphs from the email networks, and four graphs built from the economic networks.

To assign original graphs into six clusters, we first calculate the GFD and GIE vectors of all graphs using the proposed estimation method. Obviously, graphs with the same category have GFD and GIE features that are likely to be comparable. In this experiment, *Purity* is chosen as the evaluation criteria, which is a primary validation measure to determine the cluster quality. It is defined as $\sum_{i=1}^{K} \frac{m_i}{m} \max (p_{ij})$, where $K$ and $m$ are the number of clusters and the total number of members involved in the whole clustering, respectively. $p_{ij}$ denotes the probability that network $j$ is assigned to cluster $i$.

In Table VII and Table VIII, we report the quantitative results of agglomerative hierarchical graph clustering using GFD and GIE, respectively. It can be observed that the *purity* increases from 0.55 to 0.85 when we take the GIE as the input. From a numerical point of view, the estimated GFD patterns of graphs vary even if they belong to the same category. As the commonality of GFD is unreliable, and consequently cannot be applied to cluster a graph into its functional domain. The advantage of our proposed GIE lies in the exploration of both urelement and high-order properties that provide multiple perspectives for us to obtain the underlying structural information. To sum up, this experiment demonstrates that GIE can also be used in unsupervised graph clustering tasks with acceptable performance.

### Table VI

Comparisons between Greet and Other Approaches in Terms of Graph Classification Accuracy (%) on Eight Datasets Including Bioinformatics and Social Domains. The Best and the Suboptimal Results Along Each Column are Boldfaced and Underlined, Respectively.

<table>
<thead>
<tr>
<th>Clusters</th>
<th>Proteins</th>
<th>Mutag</th>
<th>Enzymes</th>
<th>COX2</th>
<th>IMDB-B</th>
<th>IMDB-Multi</th>
<th>PTC-FR</th>
<th>REDDIT-B</th>
</tr>
</thead>
<tbody>
<tr>
<td>WL [41]</td>
<td>74.32±3.13</td>
<td>87.62±5.35</td>
<td>51.30±1.67</td>
<td>76.41±6.07</td>
<td>72.89±3.93</td>
<td>50.87±3.95</td>
<td>67.64±1.74</td>
<td>81.03±3.17</td>
</tr>
<tr>
<td>Shortest-Path [42]</td>
<td>73.14±3.05</td>
<td>86.05±2.14</td>
<td>41.53±1.97</td>
<td>76.58±0.71</td>
<td>71.53±3.63</td>
<td>48.23±2.57</td>
<td>66.39±1.73</td>
<td>77.44±3.15</td>
</tr>
<tr>
<td>Graphlet [23]</td>
<td>72.58±2.46</td>
<td>85.06±2.76</td>
<td>32.55±2.78</td>
<td>78.16±1.03</td>
<td>72.63±5.49</td>
<td>47.30±3.56</td>
<td>68.57±1.04</td>
<td>80.27±4.51</td>
</tr>
<tr>
<td>DGCNN [43]</td>
<td>75.35±2.48</td>
<td>85.83±3.24</td>
<td>65.51±5.32</td>
<td>81.13±5.67</td>
<td>71.91±5.86</td>
<td>46.26±2.84</td>
<td>65.09±5.66</td>
<td>82.56±2.38</td>
</tr>
<tr>
<td>Graph-U-Nets [44]</td>
<td>77.54±2.35</td>
<td>87.21±5.57</td>
<td>69.98±4.88</td>
<td>78.17±5.81</td>
<td>75.48±3.31</td>
<td>51.88±3.88</td>
<td>66.11±6.55</td>
<td>84.37±1.57</td>
</tr>
<tr>
<td>StrucPool [45]</td>
<td>79.13±2.67</td>
<td>87.51±3.46</td>
<td>63.85±2.91</td>
<td>81.53±4.66</td>
<td>74.08±3.35</td>
<td>52.47±2.58</td>
<td>69.17±3.35</td>
<td>85.97±2.52</td>
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<tr>
<td>Bonchev. et al. [46]</td>
<td>67.35±0.17</td>
<td>82.56±0.97</td>
<td>47.31±0.88</td>
<td>73.45±1.17</td>
<td>68.77±2.02</td>
<td>48.35±1.88</td>
<td>64.73±2.12</td>
<td>80.65±2.34</td>
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<tr>
<td>Dehmer [28]</td>
<td>70.21±0.56</td>
<td>83.18±0.78</td>
<td>48.67±0.59</td>
<td>75.36±1.93</td>
<td>70.31±2.26</td>
<td>50.16±1.91</td>
<td>66.84±2.03</td>
<td>82.24±2.44</td>
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<tr>
<td>Aizl. et al. [46]</td>
<td>77.22±2.38</td>
<td>86.58±2.36</td>
<td>53.77±4.34</td>
<td>78.59±0.83</td>
<td>72.89±4.45</td>
<td>50.41±2.53</td>
<td>68.43±1.83</td>
<td>85.31±2.42</td>
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<tr>
<td>GREET (ours)</td>
<td>78.56±1.71</td>
<td>89.56±3.42</td>
<td>67.57±3.60</td>
<td>84.57±2.63</td>
<td>74.33±3.51</td>
<td>53.46±2.98</td>
<td>71.50±3.42</td>
<td>90.35±2.23</td>
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### Table VII

Quantitative Results of Agglomerative Hierarchical Graph Clustering Using GFD.

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1. The circled numbers indicate the amount of graphs assigned to each cluster.
2. $Purity = \frac{3\times1+3\times1+1\times1}{20} = 0.55$

### Table VIII

Quantitative Results of Agglomerative Hierarchical Graph Clustering Using GIE.

<table>
<thead>
<tr>
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</table>

1. $Purity = \frac{5\times1+5\times1+1\times1+4}{20} = 0.85$
V. CONCLUSION

This paper proposed GREET, a general entropy-based framework with efficient graphlet estimation algorithms for graph characterization. Firstly, an enclosing edge-centric neighborhood is constructed for exploring basic 3-, 4-vertex tree and cyclic graphlets, which leads to the high efficiency for further graphlet counting. Secondly, we propose two novel information functionals with both urelement and higher-order features considered, which are shown to be effective in understanding the structural information of networks. Then the resulting graph information entropy vector is the combination of its local and global graph entropy, which has proven its superiority in generating comprehensive network representation. Moreover, GREET also has many interchangeable parts, which enable its generalization to other applications. For example, the procedure of estimating graphlets can be replaced by alternative approaches, thus improving its flexibility and scalability. Experimental results on over twenty datasets demonstrate that our proposed method is able to calculate graphlets with high efficiency and low error, and the experiments on the graph classification task show that GREET outperforms current approaches with higher accuracy. In particular, the existing graph representation methods can also benefit from the proposed GIE in other domains.

The findings of this work give rise to many important future research directions. For instance, it would be valuable to extend the definition of local and global information functionals for directed or attribute networks. Besides, it is of great significance to measure the similarity between graph entropy and structural information so as to approximate entropies with less entropy gap. Moreover, we also intend to investigate the upper and lower bounds for the entropy measure in future work, which is still in its infancy.

REFERENCES


[42] The University of Sheffield, U.K. She has coauthored the books Fog-Enabled Intelligent IoT Systems (Springer 2020), Ultra-Dense Networks for 5G and Beyond (Wiley 2019), Heterogeneous Cellular Networks: Theory, Simulation and Deployment (Cambridge University Press 2013), and 4G Femtocells: Resource Allocation and Interference Management (Springer 2013). She was a co-recipient of the IEEE Communications Society 2017 Young Author Best Paper Award. She received the IEEE COMMUNICATIONS LETTERS Exemplary Editor Award in 2018. She is a Senior Editor for the IEEE WIRELESS COMMUNICATIONS LETTERS and an Editor for the IEEE COMMUNICATIONS LETTERS.

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