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Heterogeneous Multi-layered Network for Modeling Complex Graph-Data

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Abstract. The present paper provides a generalized model of network, namely, Heterogeneous Multi-layered Network (HMN), which can simultaneously be multi-layered and heterogeneous. We proved that the sets of all homogeneous, heterogeneous and multi-layered networks are subsets of the set of all HMNs depicting the model's generalizability. The proposed HMN is more efficient in encoding different types of nodes and edges when compared to representing the same information through heterogeneous or multilayered networks. It is found experimentally that the HMN model when used with GNNs improve tasks such as link prediction. In addition, we present a novel parameterized algorithm (with complexity analysis) for generating synthetic HMNs. The networks generated from our proposed algorithm are more consistent in modelling the layer-wise degree distribution of a real-world Twitter network (represented as HMN) than those generated by existing models. Moreover, we also show that our algorithm is more effective in modelling an air-transportation multiplex network when compared to an algorithm designed specifically for the task. Further, we define different structural measures for HMN namely multilayer neighborhood, degree centrality, closeness centrality and betweeness centrality. Accordingly, we established the equivalency of the proposed structural measures of HMNs with that of homogeneous, heterogeneous, and multi-layered networks.

Keywords: Network Science, Heterogeneous, Multilayer, Network Generation

1. Introduction

Network analysis is widely used to explain behaviors of different complex systems, ranging from physical processes to biological systems. In many cases complex systems cannot be expressed with simple networks of homogeneous nodes. Networks having diverse nodes and edges require a heterogeneous graph [39, 76, 83]. In the literature, multilayer networks have also been used for different network science problems [7, 8, 16, 62]. However, considering the nature of complex systems, it may be natural to have multiple layers, each of which contains diverse type of nodes and edges. For example, the Facebook [60] network which is heterogeneous due to different nodes like users, posts, pictures, and groups is also multi-layered due to the different relations among these nodes. A layer in Facebook can contain interactions between users based on friendship; another layer can contain relationships between users who belong to the same picture; and a third layer can be formed with interactions between users and groups. A multi-layered network cannot support heterogeneity in a layer due to the absence of node or edge types [9–11, 56]. On the other hand, a single heterogeneous network cannot retain all the information present in a multi-layered network. The existing heterogeneous networks allow only one type of link between two objects, although the network may require different links. If we use these existing data structures for the Facebook network as described, we will lose certain information. Similarly, the network of chemical, gene, pathways, and diseases (CGPD) also shows multilayer and heterogeneous characteristics [110]. However, due to the lack of modeling techniques available, in [110] the authors have used multi-relational graphs. A multirelational graph represents multiple heterogeneous graphs as a collection, and there is no way to express relations between these subgraphs. Networks with heterogeneous links between similar or different types of nodes are becoming more and more prominent in the present era. These complex networks are results of the modern internet and social networks. Furthermore, due to the availability of ActivityPub [81] protocol and the corresponding services (Fediverse [1]), which allow different social networking apps to communicate among them, we will see more heterogeneous multilayer datasets in the future. The existing data-structure has several limitations, as mentioned, to handle such complex networks. A model to represent the different semantic relationships among different entities in the form of a graph is the need of the hour.

Many networks used in different applications [43, 46, 68, 74] are not homogeneous in nature. Nevertheless, such networks are assumed to be homogeneous [27, 109], heterogeneous [52, 71] as well as multilayered [22, 47, 119] network while solving different problems. Although the combination of the words 'multilayer' and 'heterogeneous' is utilized in many of the social network research [1, 41, 65, 80, 85, 99, 100, 103, 118], these methods are merely a manifestation of the multilayer network data structure [11] in the context of application. In other words, the underlying data structure used therein does not support heterogeniety in independent layer. For example, work on sentiment analysis [41] and inter-layer coupling dynamics [85] consider each layer as homogeneous while different layers contain different types of nodes, i.e., none of the layers are heterogeneous. Nevertheless, the literature does not propose a generalized model of network that incorporates all possible characteristics of modern complex networks.

This paper proposes a new network model, generalized heterogeneous multi-layered network that can express modern complex networks, by supporting heterogeneity and multi-layered properties simultaneously. Homogeneous, heterogeneous and multilayered networks are special case of the proposed HMN. Various structural measures are developed for this network. In addition, the paper proposes a novel parameterized algorithm for generating a synthetic HMN. The algorithm is capable of generating homogeneous, heterogeneous, multilayered, and heterogeneous multilayered networks by setting the parameters appropriately. The generated network will provide different research opportunities with heterogeneous multilayer network where it is difficult to obtain a real-world data set. The paper has four main contributions as follows.

- Proposes a generalized heterogeneous multi-layered network model. We define various structural measures for this model.
- We prove that the set of all homogeneous, heterogeneous, and multilayered networks is a subset of the set of all generalized heterogeneous multilayered networks.
- We present an algorithm that generates a heterogeneous multi-layered network with various layers and different types of nodes.
- Various experimental results show the applicability of the proposed model in different applications and the benefit of incorporating layers within the model.

The remaining paper is organized as follows. In Section 2 we will briefly discuss the preliminaries, Section 3 reports the related work in the field. The proposed definition of a generalized heterogeneous multi-layered network along with its structural properties are presented in Section 4. Section 5 contains the algorithm for generating a heterogeneous multi-layered network and experimental results are presented in 7. Finally, Section 8 concludes the findings.

[1] https://fediverse.to

2. Preliminaries

Definition 2.1 (Homogeneous Networks)**.** A homogeneous network is a graph $G = (V, E)$ with the vertex set V and the edge set E denoting the relations among these vertices.

Definition 2.2 (Neighborhood)**.** The neighbourhood of a node v in a homogeneous network are the nodes that have an edge with v i.e. the neighbourhood of a node v is as defined as,

$$N(v) = \{v_j | \ (v, v_j) \in E\} \tag{1}$$

Definition 2.3 (Degree Centrality)**.** In a homogeneous network, the degree centrality (DC) of a node v is the ratio of its degree to the total number of nodes defined as,

$$DC(v) = \frac{1}{n-1}|N(v)| \tag{2}$$

Definition 2.4 (Betweenness Centrality)**.** The betweenness centrality (BC) of a node v in a homogeneous network is the fraction of the shortest paths passing through the node with the total number of shortest paths in the network. It is defined as,

$$BC(v) = \sum_{x,y \in V \setminus \{v\}} \frac{|sp(x, y|v)|}{|sp(x, y)|} \tag{3}$$

The function $sp(x, y)$ denotes the set of all shortest paths between two nodes x and y in a network and $sp(x, y|v)$ returns the shortest paths from x to y that passes through v.

Definition 2.5 (Closeness Centrality)**.** In a homogeneous network, the closeness centrality (CC) of a node v is the sum of the reciprocal of the shortest path length from v to all other nodes in the network. It is defined as,

$$CC(v) = \sum_{w \in V \setminus \{v\}} \frac{1}{distance(v, w)} \tag{4}$$

Here ($distance(v,w)$) denotes the sum of the weights on the edges of the shortest path between two nodes v and w in a network.

Definition 2.6 (Multi-layered Network [11])**.** A multi-layered network is defined as a triple $M = (Y, G_{intra}, G_{inter})$ where $Y = \{1, 2, \cdots, k\}$ is the set of layers, $G_{intra} = (G_1, G_2, G_3, ..., G_k)$ is a sequence of graphs with each graph $G_i = (V_i, E_i)$ belonging to a layer, and $G_{inter} = \{G_{ij} = (V_i, V_j, E_{ij}) | i \neq j\}$. An inter layer graph G_{ij} for layer i to j contains all the nodes and edges from layer i to layer j.

Definition 2.7 (Multiplex Network)**.** A multiplex network is a network $M = (V, E, L)$ with V as the vertex set, E as the edge set and L as the layer set. An edge in E is a tuple (x, y, l) where x, $y \in V$ and $l \in L$. The vertex set is common across the layers which allows a multiplex network to have multiple relations between the same pair of nodes with each relation captured in a different layer.

Definition 2.8 (Heterogeneous Network [91]). A network $H = (V, E, \{A, B\}, \{f_1, f_2\})$ with edges having multiple nodes and edge types with functions f_1 and f_2 to map nodes and edges respectively to their types A and B is called a heterogeneous network. It is mandatory for either the node type or the edge type to be greater than one. Two links which belong to the same relation type have the same starting node type as well as the ending node type.

3. Related Work

Heterogeneous networks have existed for a long time, with earlier work subsisting in the social sciences. One of the earlier works on heterogeneous network mining [44] explored the applications of links to mine such networks and distinguish objects based on links. The survey [91] presents a good idea about some of the more recent works on heterogeneous networks. Heterogeneous networks are seen to be applied in link prediction [71], community detection [78], modeling human collective behavior [35], rail transit network [36] and heterogeneous susceptible infected network [106].

One of the pioneering works on multi-layer networks was by Moreno et al. [56]. They have proposed a formal definition of multi-layered networks. The definition was further simplified along with the addition of structural measures in [11]. The formalism of multi-layer networks have led to various studies and applications on them. Multi-layer networks have been studied in various contexts like the study of flow processes or diffusion [17, 18], epidemic modelling and disease spreading [30, 119], generalization of the percolation theory [89, 114], clique based heuristic node analysis [53], localization properties of the network helping to understand the propagation of perturbation [50], and how the failure of nodes in one layer propagates to other layers [63]. It is essential to mention that the literature contains a wide variety of networks very similar in definition to multi-layered networks like multiplex networks [15, 57], multilevel networks [54, 115] and network of networks [75].

Heterogeneous and multilayered network models are used separately for different problems. Further, multilayer network data structure had been referred as ‘heterogeneous multilayer’ [41, 65, 80, 85, 99, 100, 103] or ‘multilayered heterogeneous’ [1, 118] when used in many applications. The probable reason for the same is to express that the whole network is heterogeneous. However, the data structures used therein do not support heterogeneity in each layer, rather can be trivially reduced to the same definition used in [56]. Hence, all these are not representative of any generalized model of networks irrespective of the nomenclatures used. Next we will highlight recent work where a multilayer network is referred to as heterogeneous multilayer network. A layered network with multiple nodes and edge types are considered heterogeneous in [41, 65, 80]. However, nodes of an individual type constitute a layer designating it as similar to multilayer network. The authors of [103] consider each type of relation to be in a separate layer, again failing to incorporate heterogeneity within a layer. Similarly, [99], considers the type of node (a person wearing a mask) to be fixed in a layer. In [1], the word heterogeneous is used to represent different non-overlapping communities in a layer. The nodes are homogeneous and, interestingly, some communities are shared between layers. This definition of layers and heterogeneity cannot be generalized to accommodate different network data.

The literature review shows us that despite having much work on heterogeneous and multi-layered networks, the literature has not addressed heterogeneity and multi-layered property simultaneously. Further, there is a requirement of data structure for network that can be used to express various types of network depending upon the problem at hand.

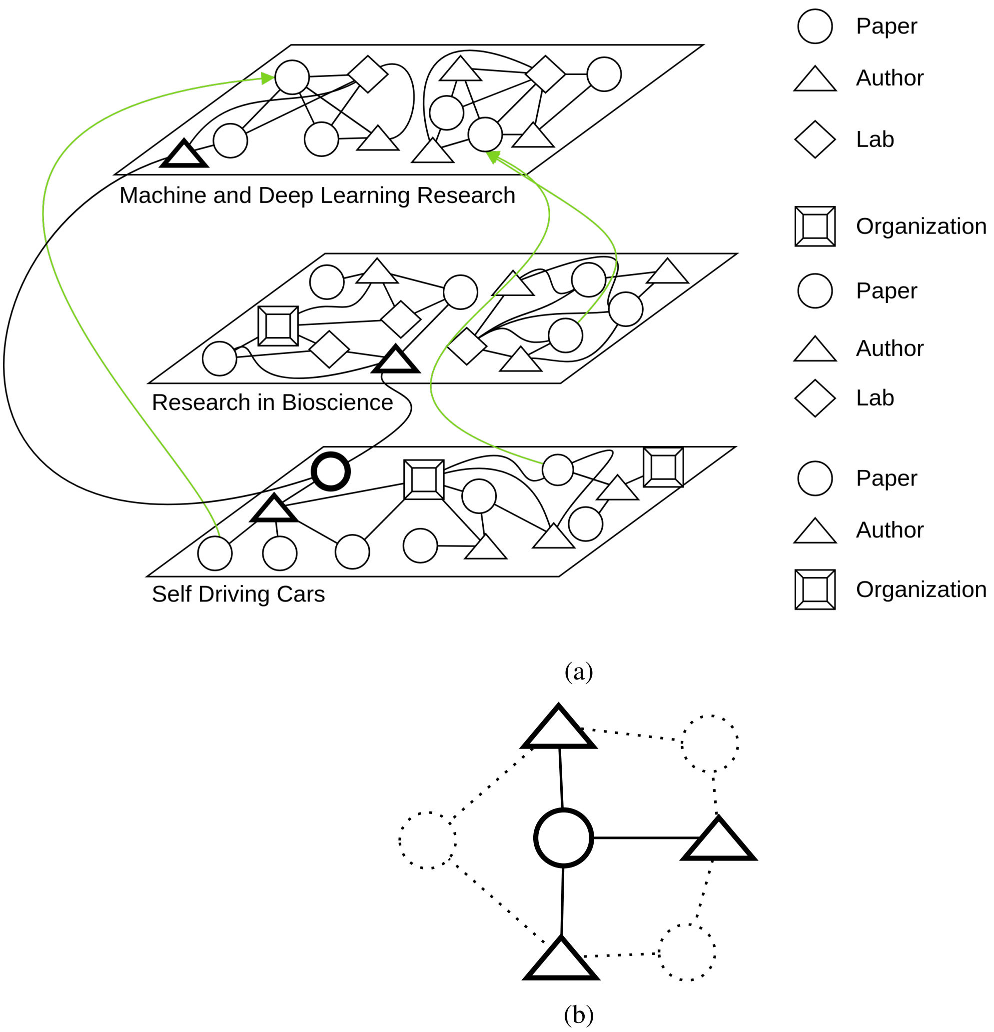


Fig. 1. a) An example to demonstrate a heterogeneous-multi-layered networks with node and edge types. In the figure the black colored edges are undirected and the green colored edges are directed. b) The figure shows the author paper relation for the authors and papers marked in bold in Figure 1(a). The circle represents paper and the triangle represents author. The dotted links and circles are the possibilities of two authors collaborating on a paper in the future.

4. Generalized Heterogeneous Multi-layered Network (HMN)

Definition 4.1 (Heterogeneous Multi-layered Network)**.** A heterogeneous-multi-layered network (HMN) is defined by quintuple $G = (V, E, L, T, \mathcal{R})$ where V is the set of vertices, $E \subseteq ((V \times L) \times (V \times L))$ is the set of edges, L is the set of layers, $T = \{T_V, T_E\}$ is the set of sets of vertex and edge types and $\mathcal{R}$ is the set of functions. $\mathcal{R}$ contains 3 primary functions R_{VT}: V $\rightarrow T_V$, R_{ET}: E $\rightarrow T_E$ to map vertex and edges to type and, R_{VL}: V $\rightarrow 2^L \setminus \{\emptyset\}$ to map a vertex to a set of layers.

A vertex may be present in many layers and cannot exist outside layers, hence the function R_{VL} maps a vertex to a power set of layers except the null set. For example a node u belonging to 3 layers l_1, l_2, l_3 will have $R_{VL}(v) = \{l_1, l_2, l_3\}$. We denote a node v at layer l as v^l for sake of convenience, i.e., $l \in R_{VL}(v^l)$. There must be at least one layer in an HMN, i.e., $|L| \geqslant 1$. The set T_V and T_E at minimum contains one type $\{\perp\}$ each.

An edge $e = (v_a^{l_b}, v_c^{l_d})$ denotes that there is a directed connection from v_a at layer l_b to v_c at layer l_d. An edge is called an intra-edge if $l_b = l_d$ or inter-edge if $l_b \neq l_d$. The set $\boldsymbol{\mathcal{R}}$ contain functions for mapping nodes and edges to their respective types and layers. The functions R_{VT} and R_{ET} map a vertex and an edge to T_V and T_E respectively.

Let us see the model with an example shown in Figure 1a. The network contains three layers with layers representing research in the machine and deep learning (Layer 1), bio-science (Layer 2), and self-driving cars (Layer 3). The figure contains three types of nodes in the Layers 1 (paper, author, lab) and 2 (paper, author, organization), and Layer 3 contains four types of nodes namely paper, author, lab, and organization. There are directed interconnections between layers to show that papers in bio-science or self-driving cars cite another paper in machine and deep learning. The network cannot be represented with a homogeneous network without losing information. Even a multi-layered or heterogeneous network will fail to capture the network due to the presence of multiple types of nodes (and edges) and multiple layers respectively. It may be apparent that a heterogeneous network will describe Figure 1a by merging different layers into one. However, a heterogeneous network only partially captures the given network as described in Remark 4.1.

Remark 4.1 (Heterogeneous Multi-Layer network is not another variant of a heterogeneous network)**.** The Figure 1a shows us in bold that three authors from three different layers have collaborated on a paper in the third layer. Consider that these three layers get merged into one, then these three authors and the paper will have the structure as shown in Figure 1b. Once we avoid the layer structure all these three authors become homogeneous. Hence there is no way to separately keep their association with each other in terms of the subjectivity expressed by the layers. For example, the possibility of collaboration between the authors of layer 1 with 3, 2 with 3 and 1 with 2 can be different. The only way we can keep this subjectivity is through the layers. Hence it is relevant to have both heterogeneity and multi-layered property in the network definition itself. This will provide a generalized definition of a complex network. We call such a network as a heterogeneous multi-layered network.

Lemma 4.1. *The set of all multi-layered networks $\mathcal{M}$ is a subset of the set of all heterogeneous multi-layered networks $\mathcal{H}_m$.*

Proof. We will prove this by contradiction. Let us assume that $\exists\ x = (Y, G_{intra}, G_{inter})$ such that $x \in \mathcal{M}$ but $x \notin \mathcal{H}_m$. Now, $\exists\ y = (V, E, L, T, \boldsymbol{\mathcal{R}}) \in \mathcal{H}_m$ such that

$$
\begin{aligned}
L &= Y \\
G(V, E) &= G_{intra} \cup G_{inter} \text{ where} \\
G_{intra} &= \{G_1, G_2, \cdots, G_k\} \text{ where } G_i = (V_i, E_i) \\
G_{inter} &= \{G_{ij}\} \text{ where } G_{ij} = (V_i, V_j, E_{ij}) \\
V_i &= \{\ v \mid v \in V \ \&\ i \in R_{VL}(v)\ \} \\
E_i &= \{\ (v_j, v_k) \mid (v_j^{l_i}, v_k^{l_i}) \in E\ \} \\
E_{ij} &= \{\ (v_k, v_m) \mid (v_k^{l_i}, v_m^{l_j}) \in E\ \}
\end{aligned}
$$

The set $V = \bigcup_{i \in L} V_i$ and $E = \bigcup_{i \in L} E_i$. Each of the graphs in a particular layer in x is homogeneous (Definition 2.1) but different layers may have different types of nodes. The functions R_{VT} and R_{ET} map all vertices and edges of a single layer to one value in the set T_V and T_E respectively. The presence of such a y using which we can create an x contradicts with our assumption. Thus we show that the set of all multi-layered networks is a subset of the set of all heterogeneous multi-layered networks. □

Corollary 4.1.1. *A multiplex network is a special case of an HMN.*

Proof. A multiplex network is a multilayered network where every layer has the same vertex set so there is no need for interconnections between the layers. In a multiplex network $M = (Y, G_{intra}, G_{inter})$, G_{intra} is $(G_1, G_2, \cdots, G_k)$ and $G_{inter} = \{G_{ij}\}$ where $G_i = (V_i, E_i)$ and $G_{ij} = (V_i, V_j, E_{ij})$ with $V_1 = V_2 = V_3 = \cdots = V_{|Y|} = V$ and $E_{ij} = \emptyset\ \forall G_{ij}$. In this case $T_V = \{T_1\}$ and $T_E = \{T'_1, \cdots, T'_{|L|}\}$. Thus a multiplex network is a special case of a multi-layered network making it a special case of an HMN. □

Lemma 4.2. *The set of all heterogeneous networks $\mathcal{H}$ is a subset of the set of all heterogeneous multi-layered networks $\mathcal{H}_m$.*

Proof. We will prove this by contradiction. Let us assume that $\exists\ x = (V_{het}, E_{het}, \{A, B\}, \{f_1, f_2\}) \in \mathcal{H}$ such that $x \notin \mathcal{H}_m$. Now, $y = (V, E, L, T, \boldsymbol{\mathcal{R}})$ with the following values for the parameters is in $\mathcal{H}_m$.

$$\begin{array}{ll} (V, E) = (V_{het}, E_{het}) & L = \{1\} \\ T_V = A & T_E = B \end{array}$$

Note that $R_{VT} \equiv f_1$ and $R_{ET} \equiv f_2$ based on the definition of heterogeneous networks. The function R_{VL} maps to default set as there is a single layer. Considering all the parameters of y are generated from the parameters of x, it is proved that for every $x \in \mathcal{H}$ there exists a corresponding $y \in \mathcal{H}_m$ such that $x \equiv y$. Thus, $x \in \mathcal{H} \implies y \in \mathcal{H}_m$ where $x \equiv y$ which shows that $\mathcal{H} \subset \mathcal{H}_m$. We use the notation $\subset$ instead of $\subseteq$ as $\mathcal{H}$ can never be equal to $\mathcal{H}_m$ due to the presence of layers in $\mathcal{H}_m$. □

Lemma 4.3. *The set of all homogeneous networks $\mathcal{S}$ is a subset of the set of all heterogeneous multi-layered networks $\mathcal{H}_m$.*

Proof. We will prove this by contradiction. Let us assume that $\exists\ x = (V_{homo}, E_{homo}) \in \mathcal{S}$ such that $x \notin \mathcal{H}_m$. Now, $y = (V, E, L, T, \boldsymbol{\mathcal{R}})$ with the following values for the parameters is in $\mathcal{H}_m$.

$$\begin{array}{ll} (V, E) = (V_{homo}, E_{homo}) & L = \{1\} \\ T_V = \{\perp\} & T_E = \{\perp\} \end{array}$$

Note that R_{VT} maps to T_V and R_{ET} maps to T_E. The function R_{VL} maps to default set as there is a single layer. Considering all the parameters of y are generated from the parameters of x, it is proved that for every $x \in \mathcal{S}$ there exists a corresponding $y \in \mathcal{H}_m$ such that $x \equiv y$. Thus, $x \in \mathcal{S} \implies y \in \mathcal{H}_m$ where $x \equiv y$ which shows that $\mathcal{S} \subset \mathcal{H}_m$. □

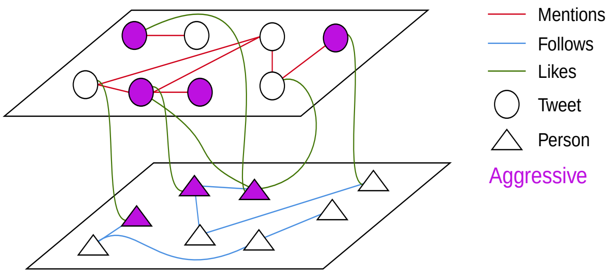


Fig. 2. An example twitter network with each rectangle representing a layer. The first layer (represented by circles) contains tweets and the second layer (represented by triangles) contains users.

It must be noted that the definition of $\mathcal{R}$ can contain additional functions. For example, all the nodes in a layer L can be returned by a function say R_{LV}, and all nodes of type T in a layer L can be returned by a function say R_{TL}. When we want all node types in a layer we can represent R_{TL} as R_L. In other words, we can add other functions to $\mathcal{R}$ as required. This makes the definition of HMN extendable for different contexts. The addition of the functions R_L and R_{TL} do not alter the definitions and proofs as mentioned earlier.

4.1. Advantages of HMN through Examples

Let us consider the network shown in the Figure 2. The network represents a real life twitter network which is heterogeneous and multi-layered at the same time. The first layer contains tweets (represented by circles). There is a connection between two tweets using the same hashtag. The second layer (represented by triangles) contains users with links between two users indicating one follows the other. In addition to that a user or tweet can be aggressive or non aggressive represented using the color. The inter-layer links represent a user liking a tweet. The above network is represented as a HMN in Figure 2. We cannot represent this information using the definitions of [10, 41, 99, 103] as there are multiple types of relations in a layer and the same node is not be present in all the layers. One may argue, that the same information can be represented as a heterogeneous network [1, 91] as shown in Figure 3, however, the complexity will increase in many folds as described here. In Figure 3 we can see that the types of nodes doubled, *i.e.*, a node can be of two types (user, tweet) where each type can have two subtypes (aggressive, non-aggressive). Now let us consider a case where a user can be mildly aggressive, moderately aggressive, severely aggressive and non-aggressive. In that case a heterogeneous network will have $2 * 4 = 8$ types of nodes and 3 types of edges making a total of 11 types to substitute 2 layers with 4 types in a HMN. It must be noted that two layers can intrinsically mean 3 types of edges (2 intra and 1 inter) without explicit markup. Similarly, increasing one layer will require $3 * 4 = 12$ node types and $3(intra) + 3(inter) = 6$ edge types in a heterogeneous network increasing the total number of types to 18 from 11. In contrast, a HMN will require 3 layers with 4 types to represent the same. In fact, a HMN intrinsically stores ${}^{|L|}C_2$ edge types which require explicit definitions in a heterogeneous network. This in-turn increases the computational complexity of certain tasks (example in the following paragraph) in a heterogeneous representation of the network. In other words, the proposed HMN model's advantage is at the abstraction level, which simplifies the data structure for complex graphs. When we compare our representation with existing representations like [80] we find that our model can store as many representations as necessary in a layer whereas existing models like MultiVERSE requires one layer for each type of node.

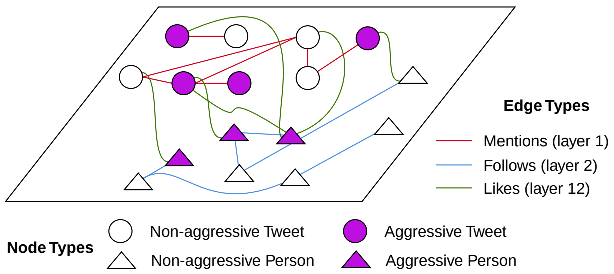


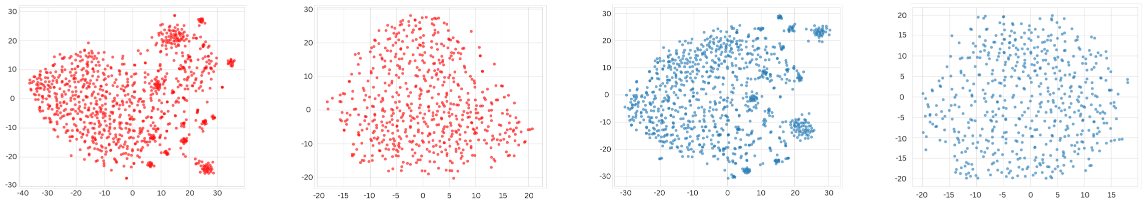
Fig. 3. An example showing twitter represented as a heterogeneous network.

Let us consider the application of HMN through the lens of link prediction in the given Twitter network. We consider the Jaccard Co-efficient for scoring a possible edge (x, y) which can be defined as $JC(x, y) = \frac{N(x) \cap N(y)}{N(x) \cup N(y)}$ where $N(x)$ defines the neighbors of node x. In a heterogeneous setting we may need to consider the neighbors of a particular type. Considering the network in Figure 3 if we need to find neighbors $N(x)$ of a particular node x of type (say tweet) we need $O(V)$ time for each node x in the worst case as shown in snippet 1 below. In the same setting, we need $O(k)$ time in our HMN with the help of function R_{TL} which returns all k vertices of a particular type in a given layer, as shown in the snippet 2. In a real Twitter network, $k << V$. We use the function R_{VL} to obtain the layer information for node x.

```
1. for n in N(x):
     if n.type == x.type:
       N_T(x).add(n)
2. for n in N(x) U R_TL(x.type, R_VL(x)):
     N_T(x).add(n)
```

4.1.1. Using layers improves existing tasks

The use of layers helps reduce types and query complexity as explained above. Now we show that layers can add additional domain knowledge to an existing heterogeneous network. In fact, we can say that a layer is meta-information about a heterogeneous network that is inherently present but not apparently visible. HMN provides a systematic way of managing this meta-information starting from the definitions to the data structure. We use the link prediction task with and without layer information on the MovieLens [45] dataset to prove our claim. MovieLens is a heterogeneous dataset with two types of nodes namely movie and user with on type of node between them namely user rates movie. There are 9742 user nodes, 610 movie nodes and 100836 edges. In the link prediction task we divide the edges in the dataset into two parts training, validation and testing. We train 2 layers GNN models like [12–14, 29, 42, 61, 72, 92, 102, 111] on the training dataset and try to predict the links on the validation and test dataset. We create two versions of the MovieLens dataset with and without layer numbers. In the version with layer numbers we encoded the domain knowledge that people who like at least one sci-fi movie rate movies differently when compared to people who like other genres of movies. We have moved sci-fi movies and users who have seen and rated at least one of them to layer 1 and other users and movies to layer 2. We encode the layer information into the feature vector by adding a bit where 0 represents layer 1 and 1 represents layer 2. In the unlayered version we use the actual feature vector which indicates all nodes belong to a single layer. We try to predict links on such a network to see what movie a user will watch (and rate) next. For the link prediction task, we use state-of-the-art GNN



(a) Movie - layer (b) User - layer (c) Movie + layer (d) User + layer

Fig. 4. Figures **a** and **b** show the t-SNE plot of the feature vector for the movie and user nodes without layer information. Figures **c** and **d** show the feature vectors after adding layer information. We can clearly see that the feature vectors have condensed after adding layer information bringing structurally similar nodes closer to one another thus increasing the result of link prediction. Features are obtained from GraphSAGE model.

architectures available. We run the GNN models on two different feature sets of the same network, the first being the feature set of the original heterogeneous network and the second with a layer dimension added to the feature vector of each movie and user. The results in Table 1 show an increase in the area under the curve for all models when we use layers. We use t-SNE (with perplexity = 30.0, learning rate of 86.26 and other parameter set to default as in the sklearn library) for reducing the dimensionality of the node features generated by our model to 2-dimensions. The t-SNE plot shown in Figure 4 shows that the embedding of movies belonging to the sci-fi genre is closer as is the embedding for the users watching that genre clearly showing the relevance of adding layers.

Table 1

AUC for the Link Prediction Task with and without layers on the movie-lens heterogeneous dataset.

Model	**Without Layer**	**With Layer**
SAGEConv [42]	92.77	**94.11**
Graphconv [72]	76.2	**80.87**
GATConv [102]	88.75	**89.77**
ResGatedGraphConv [12]	86.62	86.63
GATv2Conv [14]	89.56	**90.78**
TransformerConv [92]	92.87	**94.13**
MFConv [29]	81.89	**85.46**
GENConv [61]	93.43	**94.51**
GeneralConv [111]	77.61	**83.84**
FiLMConv [13]	75.07	**80.34**

5. Synthetic HMN Generation

It is difficult to obtain heterogeneous multi-layered network datasets despite a lot of real-world networks being HMN. We have addressed this problem by proposing a novel parameterized algorithm for generating a heterogeneous multi-layered network. The proposed algorithm can generate a multi-layered, heterogeneous, and homogeneous network using different values of the parameters as described in the Lemmas 4.1, 4.2, and 4.3 respectively.

5.1. Algorithm

The Algorithms of 1 and 2 generate an HMN. The algorithms work as follows. At time step t a new node n is added to the initially empty network G. The number of nodes that can be added to the network is limited by the parameter N. The node u is assigned to a layer l of L uniformly randomly. The type of u is assigned uniformly randomly from $R_L(l)$ where $R_L(i) = \{T_i\}_{i \in L}$ and $T_i \subseteq T_V$. Since different real-world datasets have different type distributions, we can assign node types based on any other distribution without changing any other part of the algorithm. The added node u connects with other nodes in the same layer and other layers using preferential attachment. The preference of a node is decided based on its own degree and the degree of its neighbours (Algorithm 2, Lines 6-7). This makes the algorithm capable of generating power law and other types of networks. The parameters α and β decide the weightage to be given to a node's own degree and the degree of its neighbours, respectively. The minimum number of connections a node makes with other nodes (in the same and different layers) is decided by the parameter M, a $L \times L$ matrix. For making intra-layer connections, the function *connection1* takes an induced graph G_{ii} from the HMN G where $G_{ij} = I(G, V_i \cup V_j)$. The induced graph can also be called a subHMN. An induced graph comes with all the types of nodes and edges associated with vertex set V_i in layer i and V_j in layer j. For the inter-layer connections with the node u, the function *connection2* takes three induced graphs G_{ii}, G_{jj} and G_{ij} where $i = l$ and $j \in L \setminus l$. Let us consider a situation where no nodes are in the inter-layer subHMN G_{12} and a new node (u) is assigned to the layer 1. In making a cross-layer connection with layer 2, if there are sufficient nodes ($> m_{12}$) in the layer 2, then m_{12} nodes are selected at random from layer 2 and connected with u. If the number of nodes in layer 2 $< m_{12}$, then we store the current node in a list so that the edges with u can be created once there are sufficient nodes in layer 2.

Remark 5.1. The above algorithm assigns a node to a single layer, making it incapable of generating a multiplex network without certain modifications.

5.2. Complexity Analysis and Scalability

Adding a new node in layer l triggers two functions, *conn1* and *conn2*, for intra layer and inter layer link generation. The algorithm establishes the intra layer links in $O(m)$ time where $m = M_{ll}$. Here M_{ll} denotes the minimum number of connections a node makes in its layer. Following the intra layer links, we make inter layer connections for the node with all other layers in $O(|L|m')$ considering the worst case. where $|L|$ denotes the number of layers and $m' = \max_{j \in L} (M_{lj})$. It must be noted that the worst case will arise when the node needs to connect to every other node in every layer.

6. Structural Measures of HMN

In this section, we define some of the structural measures of HMN. By definition HMN uses direction for an edge $e \in E$. However, many network measures consider the in-links and out-links together. When applicable, notations related to in-links and out-links are superscripted with IN and OUT respectively in the following text.

Definition 6.1 (Out/In-Neighborhood in HMN)**.** The Out/In-neighborhood of a node v^l is defined by the connected nodes from/to the node v^l to all the nodes situated in any layer in a set of layers $\mathcal{L}$ and having a type $t \in \mathcal{T}$. That is,

---

Algorithm 1: Generating an HMN

Input: $N, L, R_L, M, \alpha, \beta$

Output: Return HMN G

```
1  node ← 1, R_VL ← {}
2  G = Empty HMN
3  while node < N do
4      i = uniformRandom(L)
5      R_VL(node) = i
6      t = uniformRandom(R_L(i))
7      G_ii.addNode(node)
8      G_ii = connection1(G_ii, node, M_ii, α, β)
9      while j ∈ L do
10         if i ≠ j then
11             G_ij = connection2(G_ii, G_jj, G_ij, node, M_ij, α, β)
12     node = node + 1;
```

$$\begin{aligned} N^{IN}(v^l, \mathcal{L}, \mathcal{T}) = &\quad \{u^k | (u^k, v^l) \in E, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\} \\ N^{OUT}(v^l, \mathcal{L}, \mathcal{T}) = &\quad \{u^k | (v^l, u^k) \in E, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\} \end{aligned} \tag{5}$$

Remark 6.1. The definition of neighborhood is flexible to include as many types of nodes and layers we wish to take. To get all types of neighbors in all the layers we set $\mathcal{T} = T_V$ and $\mathcal{L} = L$ where T_V and L denote all vertices and layers respectively.

Remark 6.2. A node can be present in more than one layers. One should note that the definition of neighborhood presented here does not contain the neighbors that the same node v in layer k may have where $k \neq l$.

Definition 6.2 (Neighborhood in HMN)**.** The neighborhood of a node v^l is defined by $N(v^l, \mathcal{L}, \mathcal{T}) = N^{IN}(v^l, \mathcal{L}, \mathcal{T}) \cup N^{OUT}(v^l, \mathcal{L}, \mathcal{T})$.

Definition 6.3 (HMN Degree Centrality)**.** Given $\mathcal{L}$ and $\mathcal{T}$ the degree centrality (DC) of a node v^l in an HMN is the ratio of the number of neighboring nodes of v^l having type in $\mathcal{T}$ and belonging to a layer in $\mathcal{L}$ to the count of all nodes of type in $\mathcal{T}$ and any layer in $\mathcal{L}$. That is,

$$DC(v^l, \mathcal{L}, \mathcal{T}) = \frac{|N(v^l, \mathcal{L}, \mathcal{T})|}{|\{u^k | k \in \mathcal{L}, u \in V, u^k \neq v^l, R_{VT}(u) \in \mathcal{T}\}|} \tag{6}$$

Definition 6.4 (Shortest Path in HMN)**.** Given $\mathcal{L}$ and $\mathcal{T}$ the shortest path between two nodes v^l and w^k in an HMN is a path through the nodes of any layer in $\mathcal{L}$ and type in $\mathcal{T}$ such that the sum of the weights (in case of a unweighted HMN the weights of all edges are 1) of the edges in the path is minimized. There

Algorithm 2: connection1() for intra layer and connection2() for inter layer connections

```
Input: g1, g2(optional), g3(optional), node, m, α, β
G = emptyGraph()
Function nodeDistribution (G, α, β)
    nodesDist = [ ]
    for i ∈ G.nodes do
        j = 0
        c = int(α ∗ f_deg(i) + β ∗ f_neighbor_deg(i))
        while j < c do
            nodesDist.add(i)

Function connection1 (g1, node, m, α, β)
    if count(g1.nodes) < m then
        return G = g1
    if count(g1.nodes) = m then
        G = starGraph(g1.nodes)
    if g1.nodes > m then
        G.edges = g1.edges
        nodesDist = nodeDistribution(G, α, β)
        targets = uniformRandom(nodesDist, m)
        newEdges = [(node, i) | i ∈ targets]
        G.addEdges(newEdges)
    Output: return intra graph G
Function connection2 (g1, g2, g3, node, m, α, β)
    if count(g3.edges) = 0 and count(g2.nodes) < m then
        g3.add(node)
        return g3
    if count(g3.edges) = 0 then
        targets = uniformRandom(g2.nodes, m)
        for vertex ∈ g3.nodes do
            for each item in targets do
                g3.addEdge((vertex, item))

    a = g2.edges
    b = g3.edges
    a = a.add(b)
    G.addEdges(a)
    nodesDist = nodesDistribution(G, α, β)
    nodesDist = [i | i ∈ nodesDist & i ∉ g1.nodes]
    targets = uniformRandom(nodesDist, m)
    for each item in targets do
        g3.addEdge((node, item))
    Output: return inter graph g3
```

can be more than one shortest path between two nodes and the set of all such shortest paths is denoted by $sp(v^l, w^k)$. The quantity $d(v^l, w^k)$ is the sum of the weights on the edges of a shortest path between v^l and w^k. When there is no path between v^l and w^k the $d(v^l, w^k)$ is ∞.

Definition 6.5 (HMN Betweeness Centrality)**.** Given $\mathcal{L}$ and $\mathcal{T}$ the betweeness centrality of a node v^l in a heterogeneous multi-layered network is the fraction of shortest paths between any two nodes x^k and y^j (where $R_{VT}(x), R_{VT}(y) \in \mathcal{T}, k, j \in \mathcal{L}$) passing through node v^l among all the shortest paths between x^k and y^j. If there is no path between x^k and y^j then $\frac{|sp(x^k,y^j|v^l)|}{|sp(x^k,y^j)|}$ is considered to be 0. That is,

$$\begin{aligned} BC(v^l, \mathcal{L}, \mathcal{T}) &= \sum_{x^k, y^j \in V'} \frac{|sp(x^k, y^j|v^l)|}{|sp(x^k, y^j)|} \\ &\text{where } V' = \{u^i | i \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}, u \in V, u^i \neq v^l\} \end{aligned} \tag{7}$$

If we are considering only cross layered connections then we can set the *layers* variable to $L - R_{VL}(v^l)$. The cross layered betweeness will indicate the importance of a node outside its own layer.

Definition 6.6 (HMN Closeness Centrality)**.** Given $\mathcal{L}$ and $\mathcal{T}$ the closeness centrality of a node v^l in a heterogeneous multi-layered network is the average shortest path length from v^l to all other nodes of a layer in $\mathcal{L}$ and type in $\mathcal{T}$ in the network.

$$\begin{aligned} CC(v^l, \mathcal{L}, \mathcal{T}) &= \sum_{u^k \in V'} \frac{1}{d(v^l, u^k)} \\ &\text{where } V' = \{u^k | u \in V, u^k \neq v^l, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\} \end{aligned} \tag{8}$$

Lemma 6.1. *Given an HMN $G = (V, E, T, \mathcal{R})$ with $|L| = 1$ and $T_V, T_E = \{\perp\}$, i.e., when an HMN is a homogeneous network (Lemma 4.3), the neighborhood of a node $v^l \in V$ is equivalent to the neighborhood of v in a homogeneous network.*

Proof. Given HMN G is nothing but a homogeneous network as per Lemma 4.3. The Definition 6.2 considers all types of neighbors of a node v^l in all the layers when $|L| = 1, T_V, T_E = \{\perp\}$ which is nothing but the degree of the node v^1; making the neighborhood of HMN equivalent to the neighborhood of the homogeneous network (Definition 2.2) it represents. □

Corollary 6.1.1. *Given an HMN which is a homogeneous network (Lemma 6.1), $DC(v^l, \mathcal{L}, \mathcal{T})$ (Equation 6) $\equiv DC(v)$ (Equation 2) .*

Proof. The neighborhood of an HMN with parameters according to Lemma 6.1 is equivalent to the neighborhood of a homogeneous network. Thus, the numerator in Equation 6 is equivalent to the number of neighbors of a node (making numerator in Equation 6 = Equation 2). The denominator in Equation 6 contains all the nodes of the network (an HMN equivalent to a homogeneous network) except v^l (the node whose centrality we are trying to find). So, the denominator in Equation 6 is equivalent to the denominator in Equation 2. Thus, it is proved that $DC(v^l, \mathcal{L}, \mathcal{T}) \equiv DC(v)$. □

Corollary 6.1.2. *The shortest path between two nodes of an HMN with parameters* $|L| = 1, T_V, T_E = \{\perp\}$ *is equivalent to the shortest path between the same nodes in a homogeneous network.*

Proof. When we have only a single layer, i.e., $|L| = 1$ and a single type of vertex and edge , i.e., $T_V, T_E = \{\perp\}$ then we consider nodes belonging to all the layers and node types in the shortest path by default (as an HMN is a homogeneous network with the given parameters as per Lemma 4.3) making the shortest path in an HMN equivalent to the shortest path in a homogeneous network. □

Corollary 6.1.3. *Given an HMN which is a homogeneous network (Lemma 6.1),* $BC(v^l, \mathcal{L}, \mathcal{T})$ *(Equation 7)* $\equiv BC(v)$ *(Equation 3)* .

Proof. The shortest path between two nodes of an HMN with parameters as in Corollary 6.1.2 is equivalent to the shortest path between the same nodes of a homogeneous network. Thus the numerator and denominator in Equation 7 is equivalent to the numerator and denominator in Equation 3. □

Corollary 6.1.4. *Given an HMN which is a homogeneous network (Lemma 6.1),* $CC(v^l, \mathcal{L}, \mathcal{T})$ *(Equation 8)* $\equiv CC(v)$ *(Equation 4)* .

Proof. The Distance between two nodes of an HMN with parameters as in Corollary 6.1.2 is equivalent to the distance between the same nodes of a homogeneous network. Thus the numerator and denominator in Equation 8 is equivalent to the numerator and denominator in Equation 4. □

Definition 6.7 (HMN Clustering Co-efficient)**.** Given $\mathcal{L}$ and $\mathcal{T}$, the clustering coefficient (CCo) of a node, v^l, in a heterogeneous multi-layered network is defined as the fraction of triangles that the node v^l participates in, out of the total number of triangles possible through that node. That is,

$$\begin{aligned} CCo(v^l, \mathcal{L}, \mathcal{T}) &= \frac{2 * |Triangles(x^k, y^j, v^l)|}{|N(v^l, \mathcal{L}, \mathcal{T})| * (|N(v^l, \mathcal{L}, \mathcal{T})| - 1)} \\ &\text{where } k, j \in \mathcal{L}, R_{VT}(x^k) \in \mathcal{T}, R_{VT}(y^j) \in \mathcal{T} \end{aligned} \tag{9}$$

We can prove all the Lemmas and Corollary for clustering co-efficient in a similar manner as shown in the previous definitions.

7. Experiment and Results

Experiments have been performed to show the ability of the proposed algorithm to generate heterogeneous multilayered networks with structural properties close to real-world networks. We try to generate a Twitter network and an European air transportation network by changing certain parameters of our algorithm. We consider a twitter dataset as it was an example of a real life network that can be better modeled as a HMN with heterogeneity in its layers. We choose the air transportation network as it is a popular multilayer network. Further experiments are performed to compare the degree distributions and centrality measures of the generated synthetic network with their real counterparts. We report only the

Table 2

Centrality measure and clustering co-efficient of **EATN** when compared to **BINBALL** and generated HMN

Dataset	Nodes	Edges	Degree	Betweenness	Avg CC	Avg Triangles/Node	Triangles
EATN	55	97	0.06027	0.02592	0.45824	2.22683	62.62162
Generated HMN (α = 1, β = 0, M = 2)	67	208	0.06147	0.02093	0.43264	3.59262	91.1111
BINBALL	106	22	0.00388	0.0004	0.00989	0.01286	0.45455

Table 3

Comparison of Generated network with **Chemical** networks

Datasets	Nodes	Edges	Density	Avg Degree	Assortativity	Triangles	Avg Triangles/Node	Avg CC	Clique Number
ENZYMES-g272	44	156	0.165	3.55	-0.05	47	1.07	0.23	2
ENZYMES-g366	42	152	0.176	3.62	-0.03	48	1.14	0.23	1
Generated HMN (α = 0.6, β = 0.6, M = 2)	54	155	0.108	4.74	-0.06	48	1.67	0.14	4
ENZYMES-g392	48	178	0.158	3.71	-0.02	74	1.54	0.26	1
ENZYMES-g117	46	180	0.174	3.91	-0.03	59	1.28	0.19	2
Generated HMN (α = 0.7, β = 0.7, M = 2)	60	173	0.098	4.77	-0.05	65	2.25	0.17	4
ENZYMES-g526	58	220	0.133	3.79	-0.02	66	1.14	0.21	1
ENZYMES-g527	57	214	0.134	3.75	-0.03	80	1.4	0.27	2
Generated HMN (α = 0.8, β = 0.8, M = 2)	74	215	0.080	4.81	-0.028	70	2.84	0.16	4
ENZYMES-g349	64	236	0.117	3.69	0.00	78	1.22	0.24	2
ENZYMES-g103	59	230	0.134	3.9	-0.03	73	1.24	0.22	2
Generated HMN (α = 0.9, β = 0.9, M = 2)	80	233	0.074	4.82	-0.109	82	3.07	0.17	4
ENZYMES-g295	123	278	0.037	2.26	0.00	6	0.05	0.01	1
ENZYMES-g296	125	282	0.036	2.26	0.00	2	0.02	0.01	1
Generated HMN (α = 1.0, β = 1.0, M = 2)	124	258	0.034	4.16	-0.436	0	0.00	0.00	2

Table 4

Comparison of Generated network with **Biological** networks

Datasets	Nodes	Edges	Density	Avg Degree	Assortativity	Triangles	Avg Triangles/Node	Avg CC	Clique N
Bio-yeast-protein-inter	1846	4406	0.003	4.000	-0.160	72	0.110	0.050	6
Generated HMN (α = 0.7, β = 0.7, M = 2)	1978	5927	0.003	4.993	-0.800	60	0.091	0.024	4
bio-DM-HT	2989	4660	0.001	3.118	-0.090	59	0.059	0.010	3
Generated HMN (α = 0.8, β = 0.5, M = 2)	1508	4517	0.004	4.991	-0.120	68	0.135	0.019	4
bio-grid-mouse	1450	3272	0.003	4.000	-0.150	120	0.248	0.030	7
Generated HMN (α = 0.9, β = 0.7, M = 3)	1488	5939	0.005	6.983	-0.190	110	0.222	0.028	5

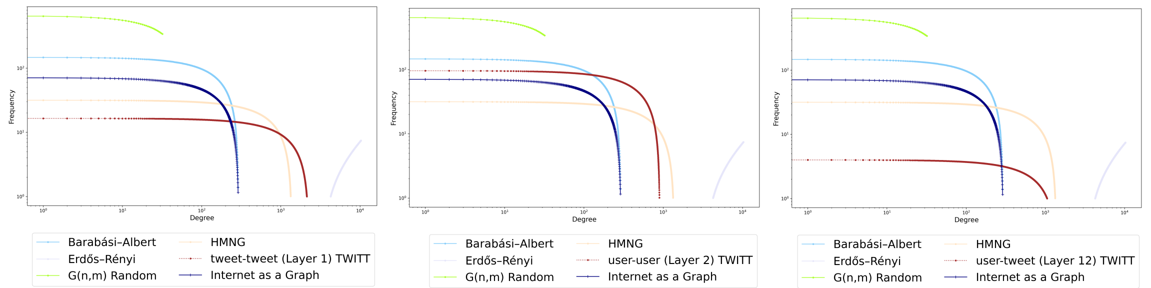
degree distribution of the nodes of both the real and synthetic network in the case of a large graph like Twitter. For the smaller air transportation network we present a comparison of the degree distributions along with other structural properties like centrality measures and clustering co-efficients. In both the cases we include comparisons with existing generation algorithms.

It must be noted that we generated an HMN with two layers for representing the real Twitter network with parameter values $L = \{1, 2\}, R_L(1) = R_L(2) = \{t_1, t_2\}$. The HMN for modelling air transportation was generated using parameter values $L = \{1, 2, ..., 37\}, R_L(i) = \{t_1\}$. We can also generate homogeneous, heterogeneous as well as multilayered networks using our proposed algorithm. In order to generate homogeneous networks we can set the values of $L = \{1\}$ and $R_L(1) = \{t_1\}$. The heterogeneous networks can be generated with $L = \{1\}, R_L(1) = \{t_1, t_2, ..., t_k\}$ and multi-layered networks can be generated with $L = \{1, 2, 3, ..., k\}, R_L(i) = \{t_1\}$ parameters. The m values for all the networks are positive samples generated from a normal distribution with a mean of 2 and a standard deviation of 1. The use of m values in this range generated degree distributions with a scale free property.

Table 5

Comparison of Generated network with **Miscellaneous** networks

Datasets	Nodes	Edges	Density	Avg Degree	Assortativity	Triangles	Avg Triangles/Node	Avg CC	Clique N
cryg2500	2500	9849	0.003	7.000	0.600	400	0.400	0.010	4
Watt-2	1856	9694	0.006	10.000	-0.070	838	0.930	0.020	4
Generated HMN (α = 1.0, β = 0.9, M = 3)	2441	9751	0.003	7.989	0.020	708	0.870	0.015	4
PTC-MR	4915	10108	0.001	4.000	-0.300	180	0.109	0.000	3
PTC-FM	4925	10110	0.001	4.000	-0.300	168	0.102	0.000	3
Generated HMN (α = 1.0, β = 0.9, M = 3)	4059	10236	0.001	5.044	-0.252	203	0.150	0.000	2
M80PI-n1	4028	8066	0.001	4.000	-0.140	0	0.000	0.000	2
S80PI-n1	4028	8066	0.001	4.000	-0.140	0	0.000	0.000	2
Generated HMN (α = 0.5, β = 0.5, M = 2)	3909	7662	0.001	3.920	-0.168	0	0.000	0.000	2
Mutag	3371	7442	0.001	4.000	-0.260	0	0.000	0.000	2
Generated HMN (α = 0.5, β = 0.5, M = 2)	3822	7338	0.001	3.840	-0.154	0	0.000	0.000	2
bn-mouse-kasthuri-graph-v4	1029	1700	0.003	3.000	-0.220	0	0.000	0.000	7
Generated HMN (α = 0.8, β = 0.5, M = 2)	807	1578	0.005	3.911	-0.259	0	0.000	0.000	2
bibd-15-3	455	1364	0.013	5.000	-0.630	166	1.094	0.010	4
Generated HMN (α = 1.0, β = 0.0, M = 3)	481	1436	0.012	5.971	-0.632	180	1.123	0.047	4
lpi-bgdbg1	629	1579	0.008	5.000	-0.040	159	0.658	0.010	3
Generated HMN (α = 1.0, β = 0.0, M = 3)	519	1550	0.012	5.973	-0.015	143	0.827	0.027	4
la-crime-moreno	829	1474	0.004	3.000	-0.160	57	0.106	0.010	3
Generated HMN (α = 1.0, β = 0.0, M = 2)	763	1443	0.005	3.782	-0.230	0	0.000	0.010	2



(a) tweet $\xleftrightarrow{\text{shares hashtag}}$ tweet layer (b) user $\xleftrightarrow{\text{follows}}$ user layer. (c) user $\xleftrightarrow{\text{posts}}$ tweet layer.

Fig. 5. Comparing the smoothed (using regression) degree distribution of the different layers of the TWITT network with our synthetic network and other standard networks on a logarithmic scale.

7.1. *A real world dataset*

We have used a Twitter dataset [40] (referred to here as *TWITT*) and represented it in the format as shown in Figure 2. We consider a twitter dataset as it was an example of a real life network that can be better modelled as a HMN with heterogenity in its layers. A tweet can be easily classified as aggressive or non-aggressive based on a standard language classification model. The Twitter network has 20125 nodes and 3938046 edges in the tweet layer (layer 1), 35936 nodes and 60824 edges in the user layer (layer 2) and 93123 edges in the user-tweet layer (interlayer connection).

7.2. *Modelling TWITT with existing generation models*

In our literature survey we have not found existing methods for generating a generic heterogeneous and multi-layered network so we compare the structural properties of the HMN generated by Algorithms 1 and 2 (referred to as HMNG here) with the existing homogeneous models. The homogeneous models used are the Barabási–Albert (BA) model [3], Erdos–Rènyi (ER) model [33], Internet as a graph [32], and G(n,m) Random graph. In each of the Figures 5a, 5b, 5c, we have compared the degree distribution of the largest component of different layers of the TWITT network with graphs generated from the aforementioned models as well as proposed synthetic network. We have generated each of these networks with number of nodes ranging from 10000 all the way to 40000 and reported the degree distribution which is most comparable to the TWITT network. For the ER model we use a p value of $0.1 - 0.9$ and report the best results. For the BA model we vary m from $2 - 5$ and report the best results (we donot use a higher m value as it does not produce comparable results). As we can see from the Figures 5a, 5b and 5c our HMNG is very close in replicating the degree distribution of the actual TWITT dataset in all the layers when compared to other modelling algorithms. For modelling the tweet-tweet and user-user layer with our HMNG we use 20000 nodes with $\alpha = \beta = 0.5$ and $m = 3$, we use $m = 4$ for the user tweet layer. The plots we use in Figure 5 are regression plots with log scale to clearly distinguish between the degree distribution of each model. It must be noted our proposed network does not have any node having a degree less than the thresholds defined in M, similar to a BA network. When we compare our results with other models we see that our model is consistent across the layers which shed light on the generic nature of our model. We have considered the interlayer as well as the intralayer degree of a node for preferential attachment, and from the Figures 5a - 5c it is evident that it well describes a real-world network.

7.3. Generating existing networks

We have successfully shown the generation capabilities of Algorithm 1 (referred to here as HMNG) for generating large heterogeneous networks with more than 10000 nodes. To demonstrate the capabilities of our proposed algorithm for generating smaller networks we have tried to model the smaller European air transportation network [15] abbreviated as $EATN$. The air transportation network is also a multiplex network having 37 different layers with each one of the layer representing a different airlines of Europe. To compare our results with existing models we have taken the BINBALL [5] generative model designed especially for modelling the multiplex air transportation network. We have generated 10 layers of the air transportation network using both BINBALL and our proposed algorithm and compared the average centrality measures of the air transportation network with both the generated networks. We generate our network with α value of 1.0, a β value of 0.0, $M = 2$ and $L = 10$ with an average of 67 nodes in a layer. For BINBALL we use the parameters as mentioned in the paper. The results are shown in Table 2. It must be noted that the results presented in Table 2 are averaged over the nodes of each of the layers in the multiplex network. The column Triangles/node denotes the average number of triangles any node participates in averaged over all the layers. In addition to the centrality measures, we compare the degree distribution of 2 layers sampled randomly from the EATN with randomly sampled layers generated from BINBALL and HMNG as shown in Figure 6 (our proposed network is referred to as HMNG). In Figure 6(a) we compare the 2nd and and 5th layers of the air transportation network with the networks generated from BINBALL and our network. In Figure 6(a) we compare the 6th and and 24th layers of the air transportation network with the networks generated from BINBALL and our network. We compare the 27th and and 13th layers of the air transportation network with the generated networks in Figure 6(c). Finally, in Figure 6(d) we compare the 2nd and and 6th layers of the air transportation network with the networks generated from BINBALL and our network. The parameters of our generated networks are according to Table 2.

The air transportation and Twitter networks alone do not represent the existing breadth of networks in the literature. To show the generalization capability of our proposed algorithm, we have tried to generate networks belonging to different domains like small molecule datasets (PTC-MR, PTC-FM), biological networks (bio-DM-HT, bio-grid-mouse, Bio-yeast-protein-inter), networks of nitroaromatic compounds (Mutag), crystal growth eigenmode graphs (cryg2500), combinatorial problems (bibd-15-3), computational fluid dynamics graph (Watt-2), linear programming problems (lpi-bgdbg1), eigenvalue model reduction problems (M80PI-n1, S80PI-n1), chemical datasets (ENZYMES-g272, g366, g392, g117, g526, g527, g349, g103, g295, g296), brain networks (bn-mouse-kasthuri-graph-v4) and even crime dataset (Ia-crime-moreno). We have collected the networks from [83]. Networks belonging to different domains have different structural properties such as degree, density, centrality measure, number of triangles and assortativity, etc. We have compared our generated network with the existing networks on such structural parameters. The results are shown in Table 3, 4, 5. We have considered other structural measures apart from centrality measures. This includes density, average degree, assortativity, triangle counts, clustering co-efficient, and the number of max cliques. It must be noted that in all the tables, CC denotes clustering coefficient.

Table 3 models Chemical Networks using Algorithm 1 with varying parameters. Except ENZYMES-295 and g296 all other networks are single layer and hence the value of L for them are kept 1. For ENZYMES-g272 and g366, we use $\alpha = \beta = 0.6$, and $M = 2$. ENZYMES-g392 and g117 use $\alpha = \beta = 0.7$, while ENZYMES-526 and g527 use $\alpha = \beta = 0.8$, both with $M = 2$. For ENZYMES-349 and g103, $\alpha = \beta = 0.9$ is used. All single-layer networks have arbitrary R_L values. ENZYMES-295 and g296 are modeled with $\alpha = \beta = 1.0$, $M = 2$, and $L = 2$, incorporating inter-layer connections, which inherently have zero triangles. In this case R_L is a function that assigns nodes to a layer uniformly randomly.

In Table 4, we model biological networks with varying parameters. For the Bio-yeast-protein-inter network, we use $\alpha = \beta = 0.7$ and $M = 2$. The bio-grid-mouse network is modeled with $\alpha = 0.9, \beta = 0.7$ and $M = 3$. For the bio-DM-HT network, we use $\alpha = 0.8, \beta = 0.5$, and $M = 2$. All networks have $L = 1$ with arbitrary R_L. Increasing M by 1 increases edge count while maintaining other network properties.

Table 5 compares various network gneerated by our methods with the network from other domains. Computational graphs (cryg2500, Watt-2) and molecule datasets (PTC-MR, PTC-FM) are generated with $\alpha = 1.0, \beta = 0.9$, $M = 3$, and $L = 1$. Graphs used in eigenvalue model reduction problems (M80PI-n1, S80PI-n1) and nitroaromatic compound (Mutag) problem is obtained by using $\alpha = \beta = 0.5$, $M = 2$, and $L = 2$, incorporating inter layer connections. Brain networks (bn-mouse-kasthuri-graph-v4) are modeled with the same parameters, totaling 807 nodes across both layers. Combinatorial problem networks (bibd-15-3) and linear programming networks (lpi-bgdbg1) use $\alpha = 1.0, \beta = 0.0$, $M = 3$, and $L = 1$. Crime dataset networks (la-crime-moreno) are represented with $\alpha = 1.0, \beta = 0.0$, $M = 2$, and $L = 1$. The total node counts for all networks are reported in Table 5. In all these cases where the number of layers $L = 2$, R_L assigns nodes to a layer uniformly randomly.

One may note that the network generation algorithm proposed in this paper is designed to have unknown node-correspondence (UNC) method [96] of generation that does not use the number of nodes and edges as identity of a network. The reason behind this is that we wanted to focus more on generating a network with same structural properties with a comparable number of nodes. It must also be noted that there is a randomness in the selection of neighbours of a node (i.e. we use a uniform distribution for selecting candidates with the same degree) which results in non-determinism, i.e. network properties may vary slightly even with the same parameter values.

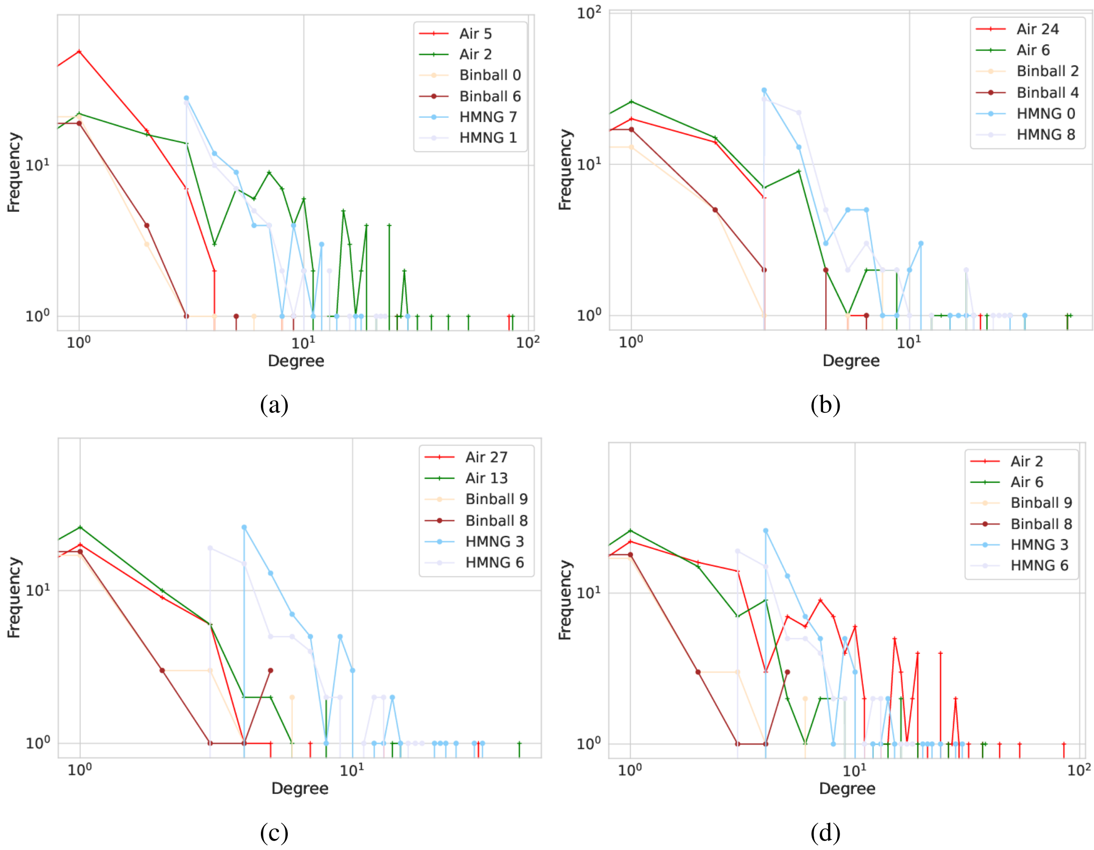


Fig. 6. The figures compare the degree distributions of randomly selected layers from EATN with networks generated from BINBALL and HMNG.

8. Discussion and Conclusion

In this paper, we introduced a new model Heterogeneous Multilayered Network (HMN), which is a generalized model of network capable of representing any complex networks of type homogeneous, heterogeneous, multilayer and their combinations. We also defined different structural measures on HMN. We have proved that the set of all HMNs is a superset of the set of all homogeneous, heterogeneous, and multi-layered networks. In addition, a parameterized algorithm is presented to generate an HMN synthetically. We show that the algorithm is able to generate a homogeneous, heterogeneous, and multilayered network by changing parameter values. Through experiments, we show that all networks generated by this algorithm have scale-free properties.

Limitations: In this work we only provided the generalized definitions of certain structural measures like degree centrality, betweeness centrality and closeness centrality. However, in network science there are many different structural properties defined for homogeneous, heterogeneous and multilayer graphs. This would be a good study to develop corresponding definitions for HMN as well. Some of these measure can be clustering co-efficient, triangles and cliques for HMN. Regarding the generation algorithm HMNG, it may not generate certain networks as it has limited number of parameters. Hence, it could only able to generate networks that is UNC with comparable node and edge counts. A better algorithm leveraging the generative capabilities of new edge GNN can be used in the future to generate synthetic graphs which can simultaneously match the numbers of nodes and edges and other structural properties of the network. Furthermore, the intra layer networks generated by our algorithm follow a scale free property now. An extension can be made to generate specific degree distribution in the future. Finally, it is of interest to find the theoretical bounds for the networks generated by our algorithm.

Despite the aforementioned limitations, the network generated by the algorithm is generalized and can be tweaked by changing the parameter values for applications in certain areas where networks largely follow a scale-free property. These synthetic networks will open the opportunity to research with HMNs that is otherwise difficult to conduct due to the unavailability of the data set. With the availability of the services (e.g., Fediverse) on ActivityPub protocol, we expect the real-world HMN data will be available in near future. Although heterogeneous network data sets are available for research, to the best of our knowledge, there is no algorithm for generating a heterogeneous network and the proposed algorithm would encourage research with heterogeneous networks as well. Note that the proposed algorithm can only be used to generate an undirected HMN. However, we believe that with minor changes, we can generate directed HMNs as well. An important future research is to show that our proposed definition of HMN holds for a dynamic network or a signed network.

Finally, with this work, we tried to open a new avenue of research with complex networks. While the theories developed will help further theoretical analysis and provide the basis of application, the synthetic network generation algorithm will provide the opportunity to develop applications with HMN.

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