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## $\frac{3}{2}$   $\mathbf{Y}$   $\mathbf{Y}$   $\mathbf{Y}$   $\mathbf{X}$   $\mathbf{Y}$   $\mathbf$ <sup>4</sup> Heterogeneous Multi-layered Network for  $5$  $\epsilon$  Modeling Complex Graph-Data  $\int_{7}^{\frac{1}{2}}$  Modeling Complex Graph-Data

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 $13$  13 14 **Abstract.** The present paper provides a generalized network model, namely, Heterogeneous Multi-layered Network (HMN), 14 <sup>15</sup> and multi-layered networks are subsets of the set of all HMNs depicting the model's generalizability. The proposed HMN is 16 more efficient in encoding different types of nodes and edges. It is found experimentally that the HMN model when used with 16  $_{17}$  GNNs improve tasks such as link prediction. In addition, we present a novel parameterized algorithm (with complexity analy-18 18 sis) for generating synthetic HMNs. The networks generated from our proposed algorithm are more consistent in modelling the <sup>19</sup> Moreover, we also show that our algorithm is more effective in modelling an air-transportation multiplex network when com-<sup>19</sup> 20 20 pared to an algorithm designed specifically for the task. Further, we define different structural measures for HMN. Accordingly,  $_{21}$  we established the equivalency of the proposed structural measures of HMNs with that of homogeneous, heterogeneous, and  $_{21}$ 22  $\sim$  22 which can simultaneously be multi-layered and heterogeneous. We proved that the sets of all homogeneous, heterogeneous layer-wise degree distribution of a real-world Twitter network (represented as HMN) than those generated by existing models. multi-layered networks.

23 23 Keywords: Network Science, Heterogeneous, Multilayer, Network Generation

## 27 **1. Introduction**  $27$

29 29 Network analysis is widely used to explain behaviors of different complex systems, ranging from <sup>30</sup> physical processes to biological systems. In many cases complex systems cannot be expressed with sim-<br><sup>30</sup> <sup>31</sup> ple networks of homogeneous nodes. Networks having diverse nodes and edges require a heterogeneous<sup>31</sup> <sup>32</sup> graph [\[39,](#page-20-0) [75,](#page-21-0) [80\]](#page-22-0). In the literature, multilayer networks have also been used for different network sci-<sup>32</sup> <sup>33</sup> ence problems [\[7,](#page-19-0) [8,](#page-19-1) [16,](#page-19-2) [62\]](#page-21-1). However, considering the nature of complex systems, it may be natural to <sup>33</sup> <sup>34</sup> have multiple layers, each of which contains diverse type of nodes and edges. For example, the Facebook<sup>34</sup> <sup>35</sup> [\[60\]](#page-21-2) network which is heterogeneous due to different nodes like users, posts, pictures, and groups is also <sup>35</sup> <sup>36</sup> multi-layered due to the different relations among these nodes. A layer in Facebook can contain inter-<br><sup>36</sup> <sup>37</sup> actions between users based on friendship; another layer can contain relationships between users who <sup>37</sup> <sup>38</sup> belong to the same picture; and a third layer can be formed with interactions between users and groups. A <sup>38</sup> <sup>39</sup> multi-layered network cannot support heterogeneity in a layer due to the absence of node or edge types. <sup>39</sup> <sup>40</sup> On the other hand, a single heterogeneous network cannot retain all the information present in a multi-<sup>40</sup> <sup>41</sup> layered network. The existing heterogeneous networks allow only one type of link between two objects, <sup>41</sup> <sup>42</sup> although the network may require different links. If we use these existing data structures for the Face-<sup>42</sup> <sup>43</sup> book network as described, we will lose certain information. Similarly, the network of chemical, gene, <sup>43</sup> <sup>44</sup> pathways, and diseases (CGPD) also shows multilayer and heterogeneous characteristics [\[104\]](#page-23-0). How-<sup>45</sup> ever, due to the lack of modeling techniques available, in [\[104\]](#page-23-0) the authors have used multi-relational<sup>45</sup> 46 46

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 1 graphs. A multirelational graph represents multiple heterogeneous graphs as a collection, and there is no 2 way to express relations between these subgraphs. Networks with heterogeneous links between similar 3 or different types of nodes are becoming more and more prominent in the present era. These complex 4 networks are results of the modern internet and social network platforms. The existing data-structure has 5 several limitations, as mentioned, to handle such complex networks. A model to represent the different <sup>6</sup> semantic relationships among different entities in the form of a graph is the need of the hour.

<sup>7</sup> Many networks used in different applications [\[43,](#page-20-1) [46,](#page-20-2) [67,](#page-21-3) [73\]](#page-21-4) are not homogeneous networks in na-<sup>8</sup> ture. Nevertheless, such networks are assumed to be homogeneous networks [\[27,](#page-19-3) [103\]](#page-22-1), heterogeneous <sup>8</sup> <sup>9</sup> networks [\[52,](#page-20-3) [70\]](#page-21-5) as well as multilayered network [\[22,](#page-19-4) [47,](#page-20-4) [113\]](#page-23-1) while solving different problems. In  $10$  some cases, authors choose to name the model as heterogeneous multilayered network but the model  $10$  $11$  implicitly uses the same definition of multi-layer network provided in [\[11\]](#page-19-5). For example, work on sen- $12$  timent analysis [\[41\]](#page-20-5) and inter-layer coupling dynamics [\[82\]](#page-22-2) consider each layer as homogeneous while  $12$ <sup>13</sup> different layers contain different types of nodes, i.e., none of the layers are heterogeneous although the <sup>13</sup> <sup>14</sup> graph is heterogeneous. A similar scenario can be found in the papers [\[95,](#page-22-3) [112\]](#page-23-2). The literature does not <sup>15</sup> propose a generic network to model all possible characteristics available in modern complex networks.<sup>15</sup>

<sup>16</sup> This paper proposes a new network model generalized heterogeneous multi-layered network that can<sup>16</sup>  $\frac{17}{10}$  express modern complex networks, i.e., the proposed model supports heterogeneity and multi-layered  $\frac{18}{10}$  property simultaneously. Various structural measures are developed for this network. In addition, the  $19$  paper proposes a novel parameterized algorithm for generating a synthetic heterogeneous multilayer  $20$  network. The algorithm is capable of generating homogeneous, heterogeneous, multilayered, and het- $20$ 21 methods. The discretion is explore of senseting homogeneous, necessarily seed, and net 21 erogeneous multilayered networks by setting the parameters appropriately. The generated network will  $\frac{22}{22}$ provide different research opportunities with heterogeneous multilayer network where it is difficult to  $\frac{1}{23}$ obtain a real-world data set. The paper has four main contributions as follows.

- <sup>25</sup> Proposes a generalized heterogeneous multi-layered network model. We define various structural <sup>25</sup> 26 measures for this model. 26
- <sup>27</sup> We prove that the set of all homogeneous, heterogeneous, and multilayered networks is a subset of <sup>27</sup> <sup>28</sup> the set of all generalized heterogeneous multilayered networks.<sup>28</sup>
- $29$  We present an algorithm that generates a heterogeneous multi-layered network with various layers  $29$ <sup>30</sup> and different types of nodes.<sup>30</sup>
- <sup>31</sup> Various experimental results show the applicability of the proposed model in different applications<sup>31</sup> <sup>32</sup> and the benefit of incorporating layers within the model.<sup>32</sup>  $\frac{33}{1}$   $\frac{1}{2}$   $\frac{1}{2}$

 34 The remaining paper is organized as follows. In Section [2](#page-1-0) we will briefly discuss the preliminaries, 35 Section [3](#page-3-0) reports the related work in the field. The proposed definition of a generalized heterogeneous 36 multi-layered network along with its structural properties are presented in Section [4.](#page-3-1) Section [5](#page-8-0) con-37 tains the algorithm for generating a heterogeneous multi-layered network and experimental results are 37 38 presented in [7.](#page-14-0) Finally, Section [8](#page-17-0) concludes the findings.

# <span id="page-1-0"></span>41 41 2. Preliminaries

<span id="page-1-1"></span>**143 Definition 2.1** (Homogeneous Networks). A homogeneous network is a graph  $G = (V, E)$  with the  $^{43}$ <br>144 vertex set V and the edge set E denoting the relations among these vertices <sup>44</sup> vertex set *V* and the edge set *E* denoting the relations among these vertices. 45 45

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- 39 39 40 40 42 42 46 46

<span id="page-2-0"></span>1 **Definition 2.2** (Neighborhood). The neighbourhood of a node *v* in a homogeneous network are the 2 2 nodes that have an edge with *v* i.e. the neighbourhood of a node *v* is as defined as,

$$
N(v) = \{v_j | (v, v_j) \in E\}
$$
\n<sup>(1)</sup>

6 6 Definition 2.3 (Degree Centrality). In a homogeneous network, the degree centrality (DC) of a node *v* 7 7 is the ratio of its degree to the total number of nodes defined as,

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

 $11$   $11$ **12 Definition 2.4** (Betweenness Centrality). The betweenness centrality (BC) of a node *v* in a homogeneous  $12$ network is the fraction of the shortest paths passing through the node with the total number of shortest  $_{13}$  $_{14}$  paths in the network. It is defined as,  $_{14}$ 

<span id="page-2-2"></span>
$$
BC(v) = \sum_{x,y \in V\backslash\{v\}} \frac{|sp(x,y|v)|}{|sp(x,y)|}
$$
\n(3)

19 19 19 19 The function  $sp(x, y)$  denotes the set of all shortest paths between two nodes *x* and *y* in a network and 19<br>20  $sp(x, y|y)$  returns the shortest paths from *x* to *y* that passes through *y*  $\frac{20}{21}$   $sp(x, y|v)$  returns the shortest paths from *x* to *y* that passes through *v*.  $\frac{20}{21}$ 

<span id="page-2-3"></span> $_{22}$  **Definition 2.5** (Closeness Centrality). In a homogeneous network, the closeness centrality (CC) of a  $_{22}$  $_{23}$  node *v* is the sum of the reciprocal of the shortest path length from *v* to all other nodes in the network. It  $_{23}$  $24$  is defined as,  $24$ is defined as,

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

<sup>29</sup> Here (*distance*(*v*,*w*)) denotes the sum of the weights on the edges of the shortest path between two <sup>29</sup>  $30$  nodes *v* and *w* in a network.

 $32$  **Definition 2.6** (Multi-layered Network [\[11\]](#page-19-5)). A multi-layered network is defined as a triple  $M = 32$  $(X, G_{intra}, G_{inter})$  where  $Y = \{1, 2, \dots, k\}$  is the set of layers,  $G_{intra} = (G_1, G_2, G_3, \dots, G_k)$  is a sequence of graphs with each graph  $G_i - (V, F_i)$  belonging to a layer and  $G_i = -fG_i - (V, V, F_i)$  is  $i \neq i$ 34 of graphs with each graph  $G_i = (V_i, E_i)$  belonging to a layer, and  $G_{inter} = \{G_{ij} = (V_i, V_j, E_{ij}) | i \neq j\}$ .<br>An inter layer graph  $G_i$  for layer *i* to *i* contains all the podes and edges from layer *i* to layer *i* 35 An inter layer graph  $G_{ij}$  for layer *i* to *j* contains all the nodes and edges from layer *i* to layer *j*.

 $\frac{36}{26}$  per executive  $\frac{36}{26}$  is the set of  $\frac{36}{26}$  in  $\frac{36}{26}$  in  $\frac{36}{26}$ **Definition 2.7** (Multiplex Network). A multiplex network is a network  $M = (V, E, L)$  with *V* as the state of *F* as the edge set and *L* as the layer set. An edge in *F* is a tuple  $(x, y, l)$  where  $x, y \in V$  and 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  $l \in I$ . The vertex set is common across the layers which allows a multiplex network to have multiple  $l \in L$ . The vertex set is common across the layers which allows a multiplex network to have multiple  $\frac{39}{39}$ relations between the same pair of nodes with each relation captured in a different layer.

**11 Definition 2.8** (Heterogeneous Network [\[88\]](#page-22-4)). A network  $H = (V, E, \{A, B\}, \{f_1, f_2\})$  with edges hav-<br><sup>42</sup> ing multiple nodes and edge types with functions  $f_1$  and  $f_2$  to man nodes and edges respectively to their <sup>42</sup> ing multiple nodes and edge types with functions  $f_1$  and  $f_2$  to map nodes and edges respectively to their <sup>42</sup> <sup>43</sup> types *A* and *B* is called a heterogeneous network. It is mandatory for either the node type or the edge  $43$ <sup>44</sup> type to be greater than one. Two links which belong to the same relation type have the same starting <sup>44</sup> <sup>45</sup> and type as well as the ending node type. <sup>45</sup> 46 46

<span id="page-2-1"></span>

 $2 \times 2$ 

## $1$  3. Related Work  $1$

 3 In the literature heterogeneous and multilayered network models are used separately for different 4 social network analysis problems. A multilayered network with nodes for keyword, hashtag, and mention 5 types is used for sentiment analysis [\[41\]](#page-20-5). The authors consider that their network is heterogeneous due 6 to the presence of multiple types of nodes, but each layer of the network was homogeneous. In other 7 words, the network is just a simple multilayered network according to the definition of [\[10\]](#page-19-6). Except this 8 work, there is no mention of heterogeneous multilayered networks in the literature.

<sup>9</sup> One of the pioneering works on multi-layer networks was by [\[56\]](#page-21-6). They have proposed a formal <sup>10</sup> definition of multi-layered networks. The definition was further simplified along with the addition of <sup>10</sup> <sup>11</sup> structural measures in [\[11\]](#page-19-5). The formalism of multi-layer networks have led to various studies and <sup>11</sup> <sup>12</sup> applications on them. Multi-layer networks have been studied in various contexts like the study of flow <sup>12</sup> <sup>13</sup> processes or diffusion [\[17,](#page-19-7) [18\]](#page-19-8), epidemic modelling and disease spreading [\[30,](#page-20-6) [113\]](#page-23-1), generalization of <sup>13</sup> <sup>14</sup> the percolation theory [\[86,](#page-22-5) [108\]](#page-23-3), clique based heuristic node analysis [\[53\]](#page-20-7), localization properties of <sup>14</sup> <sup>15</sup> the network helping to understand the propagation of perturbation [\[50\]](#page-20-8), and how the failure of nodes<sup>15</sup> <sup>16</sup> in one layer propagates to other layers [\[63\]](#page-21-7). It is essential to mention that the literature contains a wide <sup>16</sup> <sup>17</sup> variety of networks very similar in definition to multi-layered networks like multiplex networks [\[15,](#page-19-9) [57\]](#page-21-8), <sup>17</sup> <sup>18</sup> multilevel networks [\[54,](#page-20-9) [109\]](#page-23-4) and network of networks [\[74\]](#page-21-9).

<sup>19</sup> Heterogeneous networks have existed for a long time with earlier works subsisting in social sciences.<sup>19</sup> <sup>20</sup> The paper [\[44\]](#page-20-10) is one of the earlier works in heterogeneous network mining exploring the applications of <sup>20</sup> <sup>21</sup> links to mine such networks and distinguish objects based on links. The survey [\[88\]](#page-22-4) presents a good idea <sup>21</sup> <sup>22</sup> about some of the more recent works on heterogeneous networks. Heterogeneous networks are seen to <sup>22</sup> <sup>23</sup> be applied in link prediction [\[70\]](#page-21-5), community detection [\[77\]](#page-21-10), modeling human collective behavior [\[35\]](#page-20-11), <sup>23</sup> <sup>24</sup>  $\alpha$  rail transit network [\[36\]](#page-20-12) and heterogeneous susceptible infected network [\[100\]](#page-22-6).

<sup>25</sup> 25 25 The literature review shows us that despite having much work on heterogeneous and multi-layered<sup>25</sup> <sup>26</sup> networks, the literature has not addressed heterogeneity and multi-layered property simultaneously.<sup>26</sup> 27 and 2012 and 201

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## <span id="page-3-1"></span><sup>29</sup> **4. Generalized Heterogeneous Multi-layered Network (HMN)**  $^{29}$  **29**  $30$   $30$

 $31$  **Definition 4.1** (Heterogeneous Multi-layered Network). A heterogeneous-multi-layered network (HMN)  $31$ <sup>32</sup> 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<br><sup>33</sup> the set of edges *L* is the set of layers  $T = {T_V, T_S}$  is the set of sets of vertex and edge types and **R**<sup>33</sup> 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  $\mathcal{R}$  <sup>33</sup><br><sup>34</sup> is the set of functions **R** contains 3 primary functions  $R_{VT}$ ;  $V \to T_V$ ,  $R_{TT}$ ;  $F \to T_E$  to man is the set of functions. R contains 3 primary functions  $R_{VT}$ : V  $\rightarrow T_V$ ,  $R_{ET}$ : E  $\rightarrow T_E$  to map vertex and <sup>34</sup> edges to type and,  $R_{VL}: V \to 2^L \setminus \{ \emptyset \}$  to map a vertex to a set of layers.  $36$  31  $\frac{3}{2}$   $\frac{3}{2}$  36

37 37 A vertex may be present in many layers and cannot exist outside layers, hence the function *RVL* maps a <sup>38</sup> 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 <sup>38</sup><br><sup>39</sup> have  $R_{11}(y) = l_1, l_2, l_3$  We denote a node *y* at layer *l* as  $y^l$  for sake of conveni 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.,  $l \in R_{VL}(v^l)$ . <sup>39</sup><br>40 There must be at least one layer in an HMN i.e.  $|I| > 1$  The set  $T_v$  and  $T_v$  at minimum con There must be at least one layer in an HMN, i.e.,  $|L| \ge 1$ . The set  $T_V$  and  $T_E$  at minimum contains one <sup>40</sup>  $41$  type  $\{\perp\}$  each.  $41$ 

<sup>42</sup> An edge  $e = (v_a^b, v_c^{\prime d})$  denotes that there is a directed connection from  $v_a$  at layer  $l_b$  to  $v_c$  at layer  $l_d$ . An <sup>42</sup><br><sup>43</sup> edge is called an intra-edge if  $l_c = l$  or inter-edge if  $l_c \neq l_c$ . The set **R** contain <sup>43</sup> edge is called an intra-edge if  $l_b = l_d$  or inter-edge if  $l_b \neq l_d$ . The set **R** contain functions for mapping <sup>43</sup>  $^{44}$  nodes and edges to their respective types and layers. The functions  $R_{VT}$  and  $R_{ET}$  map a vertex and an  $^{44}$  $^{45}$  edge to  $T_V$  and  $T_E$  respectively. 46 46

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<span id="page-4-0"></span>

 authors and papers marked in bold in Figure [1\(a\)](#page-4-0). The circle represents paper and the triangle represents author. The dotted  $34$ 35 links and circles are the possibilities of two authors collaborating on a paper in the future.

37 Let us see the model with an example shown in Figure [1a.](#page-4-0) The network contains three layers with 37 38 layers representing research in the machine and deep learning (Layer 1), bio-science ( Layer 2), and 39 self-driving cars (Layer 3). The figure contains three types of nodes in the Layers 1 (paper, author, lab) 40 and 2 (paper, author, organization), and Layer 3 contains four types of nodes namely paper, author, lab, <sup>41</sup> and organization. There are directed interconnections between layers to show that papers in bio-science <sup>41</sup> <sup>42</sup> or self-driving cars cite another paper in machine and deep learning. The network cannot be represented <sup>42</sup> <sup>43</sup> with a homogeneous network without losing information. Even a multi-layered or heterogeneous net-<br><sup>43</sup> <sup>44</sup> work will fail to capture the network due to the presence of multiple types of nodes (and edges) and <sup>44</sup> <sup>45</sup> multiple layers respectively. It may be apparent that a heterogeneous network will describe Figure [1a](#page-4-0) by 46

1 merging different layers into one. However, a heterogeneous network only partially captures the given 1 2 2 network as described in Remark [4.1.](#page-5-0)

<span id="page-5-0"></span> $3$ **Remark 4.1** (Heterogeneous Multi-Layer network is not another variant of a heterogeneous network).  $_{5}$  The Figure [1a](#page-4-0) shows us in bold that three authors from three different layers have collaborated on a  $_{5}$  $6<sub>6</sub>$  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.](#page-4-0) Once we avoid the layer structure all these  $\frac{1}{7}$  $8<sub>8</sub>$  three authors become homogeneous. Hence there is no way to separately keep their association with each  $8<sub>8</sub>$ <sup>9</sup> 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  $_{10}$ this subjectivity is through the layers. Hence it is relevant to have both heterogeneity and multi-layered  $_{11}$  $_{12}$  property in the network definition itself. This will provide a generalized definition of a complex network.  $13$  We call such a network as a heterogeneous multi-layered network.

<span id="page-5-1"></span>14 14 **Lemma 4.1.** The set of all multi-layered networks M is a subset of the set of all heterogeneous multi-<br><sup>15</sup>  $\frac{16}{16}$   $\frac{16}{16}$   $\frac{16}{16}$   $\frac{16}{16}$ *layered networks* H*m.*

- 17 **n**  $\mathbf{a}$  w  $\mathbf{u}$  is the  $\mathbf{v}$  in  $\mathbf{v}$  and  $\mathbf{v}$  and  $\mathbf{u}$  is  $\mathbf{u}$  and  $\mathbf{v}$  is  $\mathbf{u}$  is  $\mathbf{u}$  is  $\mathbf{v}$  is  $\mathbf{u}$  is  $\mathbf{v}$  is  $\mathbf{u}$  is  $\mathbf{v}$  is  $\mathbf{v}$  is  $\mathbf{v}$  is  $\mathbf$ **Proof.** We will prove this by contradiction. Let us assume that  $\exists x = (Y, G_{intra}, G_{inter})$  such that  $x \in \mathcal{M}$  18 but  $x \notin \mathcal{H}_m$ . Now,  $\exists y = (V, E, L, T, \mathcal{R}) \in \mathcal{H}_m$  such that
- 20  $\qquad \qquad$  20 21  $\overline{21}$  21  $\overline{21}$  21 22  $G(V, E) = G_{intra} \cup G_{inter}$  where 22  $G_{intra}$   $G_{intra}$   $= \{G_1, G_2, \cdots, G_k\}$  where  $G_i = (V_i, E_i)$   $=$   $\frac{23}{24}$  $24$   $24$   $24$   $24$ 25  $G_{\text{inter}} = \{G_{ij}\}\text{ where } G_{ij} = (V_i, V_j, E_{ij})$ <br>25  $G_{\text{inter}} = \{G_{ij}\}\text{ where } G_{ij} = \{V_i, V_j, E_{ij}\}\$ 26  $V_i = \{ v \mid v \in V \& i \in R_{VL}(v) \}$ 27 and  $(1 - 2)$  27 28  $E_i$   $= \{ (v_j, v_k) | (v_j^{l_i}, v_k^{l_i}) \in E \}$  28  $29$  $E_{ij} = \{ (v_k, v_m) | (v_k^{l_i}, v_m^{l_j}) \in E \}$  $L = Y$

 $31$   $31$ 

33 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 33  $34$  (Definition [2.1\)](#page-1-1) but different layers may have different types of nodes. The functions  $R_{VT}$  and  $R_{ET}$  map  $34$ <sup>35</sup> all vertices and edges of a single layer to one value in the set  $T_V$  and  $T_E$  respectively. The presence of <sup>35</sup> <sup>36</sup> such a *y* using which we can create an *x* contradicts with our assumption. Thus we show that the set of <sup>36</sup> <sup>37</sup> all multi-layered networks is a subset of the set of all heterogeneous multi-layered networks.  $\Box$ <sup>37</sup>

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40 40

# 39 39 Corollary 4.1.1. *A multiplex network is a special case of an HMN.*

<sup>41</sup> Proof. A multiplex network is a multilayered network where every layer has the same vertex set so <sup>41</sup> there is no need for interconnections between the layers. In a multiplex network  $M = (Y, G_{intra}, G_{inter})$ , <sup>42</sup><br><sup>43</sup>  $G_{i,j}$  is  $(G_1, G_2, \ldots, G_k)$  and  $G_{i,j} = \{G_{i,j}\}$  where  $G_i = (V, F_i)$  and  $G_{i,j} = (V, V, F_{i,j})$  with  $V_i =$  <sup>43</sup> <sup>43</sup>  $G_{intra}$  is  $(G_1, G_2, \dots, G_k)$  and  $G_{inter} = \{G_{ij}\}\$  where  $G_i = (V_i, E_i)$  and  $G_{ij} = (V_i, V_j, E_{ij})$  with  $V_1 =$ <br><sup>44</sup>  $V_2 = V_2 = \dots = V_{i,j} = V$  and  $F_i = \emptyset$   $\forall G_i$ . In this case  $T_i = \{T_i\}$  and  $T_i = \{T'_i\}$ ,  $T'_i \ge T'_i$  Thus a <sup>44</sup>  $V_2 = V_3 = \cdots = V_{|Y|} = V$  and  $E_{ij} = \emptyset \ \forall G_{ij}$ . In this case  $T_V = \{T_1\}$  and  $T_E = \{T'_1, \cdots, T'_{|L|}\}\)$ . Thus a  $^{44}$ <br><sup>45</sup> multiplex petycrk is a special case of a multi-layered petycrk making it a special case of an H <sup>45</sup> multiplex network is a special case of a multi-layered network making it a special case of an  $\text{HMN}$ .  $\square$ <sup>45</sup> 46 46

<span id="page-6-0"></span>1 **Lemma 4.2.** The set of all heterogeneous networks H is a subset of the set of all heterogeneous multi-<br>1 2 2 *layered networks* H*m.*

**Proof.** We will prove this by contradiction. Let us assume that  $\exists x = (V_{het}, E_{het}, \{A, B\}, \{f_1, f_2\}) \in \mathcal{H}$  and the total in  $\forall x$  = (*V*  $F \in \mathcal{F} \cap \mathcal{F}$ ) with the following values for the parameters is in  $\mathcal{H}$ 5 such that *x* ∉  $\mathcal{H}_m$ . Now, *y* = (*V*, *E*, *L*, *T*, **R**) with the following values for the parameters is in  $\mathcal{H}_m$ .

$$
T_V = A
$$
  
\n
$$
T_V = A
$$
  
\n
$$
T_E = B
$$
  
\n
$$
T_E = B
$$
  
\n
$$
T_V = 0
$$
  
\n<math display="</math>

en de la construction de la constr<br>De la construction de la construct 10 Note that  $R_{VT} \equiv f_1$  and  $R_{ET} \equiv f_2$  based on the definition of heterogeneous networks. The function 10  $R_{VL}$  maps to default set as there is a single layer. Considering all the parameters of *y* are generated from  $11$ 12 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 13  $x \equiv y$ . Thus,  $x \in \mathcal{H}$  ⇒  $y \in \mathcal{H}_m$  where  $x \equiv y$  which shows that  $\mathcal{H} \subset \mathcal{H}_m$ . We use the notation ⊂ 13 instead of ⊆ as H can never be equal to  $\mathcal{H}_m$  due to the presence of layers in  $\mathcal{H}_m$ . □

<span id="page-6-1"></span>15 15 16 **Lemma 4.3.** The set of all homogeneous networks  $S$  is a subset of the set of all heterogeneous multi- $\mu_{17}$  layered networks  $\mathcal{H}_m$ .

18 <u>is a comparative contract the set of the s</u> **Proof.** We will prove this by contradiction. Let us assume that  $\exists x = (V_{homo}, E_{homo}) \in S$  such that  $\tau \notin H$  Now  $y = (V F I T \mathcal{R})$  with the following values for the parameters is in  $H$  $x \notin \mathcal{H}_m$ . Now,  $y = (V, E, L, T, \mathcal{R})$  with the following values for the parameters is in  $\mathcal{H}_m$ .

$$
T_V = \{L\}
$$
  
\n
$$
T_V = \{\perp\}
$$
  
\n
$$
T_E = \{\perp\}
$$

24 24 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  $26$   $\frac{3}{26}$   $\frac{1}{26}$   $\frac{1}{2$ for every  $x \in S$  there exists a corresponding  $y \in \mathcal{H}_m$  such that  $x \equiv y$ . Thus,  $x \in S \implies y \in \mathcal{H}_m$  where  $x \equiv y$  which shows that  $S \subset \mathcal{H}_m$ . □ single layer. Considering all the parameters of *y* are generated from the parameters of *x*, it is proved that

<sup>29</sup> It must be noted that the definition of **R** can contain additional functions. For example, all the nodes  $\frac{30}{21}$  in a layer *L* can be returned by a function say  $R_L$ <sub>V</sub>, and all nodes of type *T* in a layer *L* can be returned by  $R_{TL}$  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, <sup>32</sup> we can add other functions to  $\pi$  as required. This makes the definition of HMN extendable for different  $\frac{33}{28}$   $\frac{3$ contexts. The addition of the functions  $R_L$  and  $R_{TL}$  do not alter the definitions and proofs as mentioned  $35$  35  $35$ earlier.

## 36 36 *4.1. Advantages of HMN through Examples*  $37$   $37$

<sup>38</sup> Let us consider the network shown in the Figure [2.](#page-7-0) The network represents a real life twitter network<sup>38</sup> <sup>39</sup> which is heterogeneous and multi-layered at the same time. The first layer contains tweets. There is <sup>39</sup> <sup>40</sup> a connection between two tweets using the same hashtag. The second layer contains users with links <sup>40</sup> <sup>41</sup> between two users indicating one follows the other. In addition to that a user or tweet can be aggressive <sup>41</sup> <sup>42</sup> or non aggressive represented using the color. The inter-layer links represent a user liking a tweet. The <sup>42</sup>  $43$  above network is represented as a HMN in Figure [2.](#page-7-0) One may argue, that the same information can be  $43$ <sup>44</sup> represented as a heterogeneous network (in Figure [3\)](#page-7-1), however, the complexity will increase in many <sup>44</sup> folds as described here. In Figure [3](#page-7-1) we can see that the types of nodes doubled, *i.e.*, a node can be of  $\frac{45}{46}$ 46 46

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<span id="page-7-1"></span>

 $21$  Fig. 3. An example twitter network with each rectangle representing a layer. The first layer contains tweets and the second layer  $21$ 22 contains users. 22 contains users.

 $23$  23

<sup>24</sup> two types (user, tweet) where each type can have two subtypes (aggressive, non-aggressive). Now let us <sup>24</sup> <sup>25</sup> consider a case where a user can be mildly aggressive, moderately aggressive, severely aggressive and <sup>25</sup> <sup>26</sup> non-aggressive. In that case a heterogeneous network will have  $2 * 4 = 8$  types of nodes and 3 types of <sup>26</sup> <sup>27</sup> edges making a total of 11 types to substitute 2 layers with 4 types in a HMN. It must be noted that two <sup>27</sup> <sup>28</sup> layers can intrinsically mean 3 types of edges (2 intra and 1 inter) without explicit markup. Similarly, <sup>28</sup> 29 increasing one layer will require  $3 * 4 = 12$  node types and  $3(intra) + 3(inter) = 6$  edge types in a <sup>29</sup>  $\frac{30}{10}$  heterogeneous network increasing the total number of types to 18 from 11. In contrast, a HMN will  $\frac{30}{10}$ <sup>31</sup> require 3 layers with 4 types to represent the same. In fact, a HMN intrinsically stores  $|L|C_2$  edge types  $\frac{32}{22}$  which require explicit definitions in a heterogeneous network. This in-turn increases the computational 33 minimized explore definitions in a necession contract this in tail increases the compatitional complexity of certain tasks (example in the following paragraph) in a heterogeneous representation of  $\frac{34}{34}$  $35$  the network. In other words, the proposed HMN model's advantage is at the abstraction level, which  $35$ 36 36 simplifies the data structure for complex graphs.

 $37$  Let us consider the application of HMN through the lens of link prediction in the given Twitter net-38 work. We consider the Jaccard Co-efficient for scoring a possible edge  $(x, y)$  which can be defined as work. We consider the Jaccard Co-efficient for scoring a possible edge  $(x, y)$  which can be defined as<br>39  $JC(x, y) = \frac{N(x) \cap N(y)}{N(x) \cup N(y)}$  where  $N(x)$  defines the neighbors of node x. In a heterogeneous setting we may 40 40 need to consider the neighbors of a particular type. Considering the network in Figure [3](#page-7-1) if we need to 41 find neighbors  $N(x)$  of a particular node x of type (say tweet) we need  $O(V)$  time for each node x in the 41 42 worst case as shown in snippet 1 below. In the same setting, we need  $O(k)$  time in our HMN with the 42 <sup>43</sup> help of function  $R_{TL}$  which returns all *k* vertices of a particular type in a given layer, as shown in the 44 snippet 2. In a real Twitter network,  $k \ll V$ . We use the function  $R_{VL}$  to obtain the layer information for  $\frac{44}{15}$  node *r*  $\frac{45}{45}$  node r  $\frac{45}{45}$ 46 46  $JC(x, y) = \frac{N(x) \cap N(y)}{N(x) \cup N(y)}$  where  $N(x)$  defines the neighbors of node *x*. In a heterogeneous setting we may need to consider the neighbors of a perticular type. Considering the network in Figure 3 if we need to node *x*.

<span id="page-7-0"></span>



10 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 10  $c$  and **d** show the feature vectors after adding layer information. We can clearly see that the feature vectors have condensed after  $11$ <sup>12</sup> Features are obtained from GraphSAGE model. <sup>12</sup><sup>12</sup> adding layer information bringing structurally similar nodes closer to one another thus increasing the result of link prediction.

```
14 1. for n in N(x):
15 15
if n.type == x.type:
N_T(x).add(n) 1617 2. for n in N(x) U R_{TL}(x, type, R_{VL}(x)):<br>
18 N_{-L}(x) add(n)
N_T(x).add(n) 18
```
# 21 21 *4.1.1. Using layers improves existing tasks*

<sup>22</sup> 22 The use of layers helps reduce types and query complexity as explained above. Now we show that <sup>22</sup> <sup>23</sup> layers can add additional domain knowledge to an existing heterogeneous network. In fact, we can <sup>23</sup> <sup>24</sup> say that a layer is meta-information about a heterogeneous network that is inherently present but not <sup>24</sup> <sup>25</sup> apparently visible. HMN provides a systematic way of managing this meta-information starting from <sup>25</sup> <sup>26</sup> the definitions to the data structure. To prove our claim, we have taken the movie lens dataset [\[45\]](#page-20-13) and <sup>26</sup>  $27$  encoded the domain knowledge that people who like at least one sci-fi movie rate movies differently  $27$ <sup>28</sup> when compared to people who like other genres of movies. We have moved sci-fi movies and users who <sup>28</sup> <sup>29</sup> have seen and rated at least one of them to layer 1 and other users and movies to layer 2. We try to predict <sup>30</sup> links on such a network to see what movie a user will watch (and rate) next. For the link prediction task, <sup>31</sup> we use state-of-the-art GNN architectures available. We run the GNN models on two different feature<sup>31</sup> <sup>32</sup> sets of the same network, the first being the feature set of the original heterogeneous network and the <sup>32</sup> <sup>33</sup> second with a layer dimension added to the feature vector of each movie and user. The results in Table [1](#page-9-0)<sup>33</sup> <sup>34</sup> show an increase in the area under the curve for all models when we use layers. The t-SNE plot shown in<sup>34</sup> <sup>35</sup> 35 <sup>35</sup> 35 <sup>35</sup> 35 <sup>35</sup> 35 <sup>35</sup> 35 Eigure [4](#page-8-1) shows that the embedding of movies belonging to the sci-fi genre is closer as is the embedding  $\frac{36}{25}$  for the users watching that genre clearly showing the relevance of adding layers.  $\frac{37}{37}$  37

## <span id="page-8-0"></span><sup>39</sup> 5. Synthetic HMN Generation **39** 39 40 40

<sup>41</sup> It is difficult to obtain heterogeneous multi-layered networks despite a lot of real-world networks be-<sup>41</sup>  $^{42}$  ing HMN. We have addressed this problem by proposing a novel parameterized algorithm for generating  $^{42}$ <sup>43</sup> a heterogeneous multi-layered network. The proposed algorithm can generate a multi-layered, heteroge-<sup>43</sup> <sup>44</sup> neous, and homogeneous network using different values of the parameters as described in the Lemmas <sup>44</sup> 45 45 [4.1,](#page-5-1) [4.2,](#page-6-0) and [4.3](#page-6-1) respectively.

46 46

<span id="page-8-1"></span>en de la construction de la constr<br>De la construction de la construct  $13$  13  $19$  and  $19$  $20$  20 38 38

<span id="page-9-0"></span>

 $15$  15

#### $\frac{14}{14}$   $\frac{1}{14}$   $\frac{1}{14}$   $\frac{1}{14}$ *5.1. Algorithm*

16 16 The Algorithms of [1](#page-10-0) and [2](#page-11-0) generate an HMN. The algorithms work as follows. At time step *t* a <sup>17</sup> new node *n* is added to the initially empty network *G*. The number of nodes that can be added to the <sup>18</sup> 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 20 different real-world datasets have different type distributions, we can assign node types based on any 20 <sup>21</sup> other distribution without changing any other part of the algorithm. The added node *u* connects with  $\frac{21}{2}$ <sup>22</sup> other nodes in the same layer and other layers using preferential attachment. The preference of a node  $\frac{23}{100}$  is decided based on its own degree and the degree of its neighbours (Algorithm [2,](#page-11-0) Lines 6-7). This  $24$  makes the algorithm capable of generating power law and other types of networks. The parameters  $24$ <sup>25</sup> *α* and *β* decide the weightage to be given to a node's own degree and the degree of its neighbours,<br><sup>26</sup> respectively. The minimum number of connections a node makes with other nodes (in the same and <sup>26</sup>  $\frac{26}{25}$  respectively. The minimum number of connections a node makes with other nodes (in the same and  $\frac{26}{27}$  $^{27}$  different layers) is decided by the parameter *M*, a  $L \times L$  matrix. For making intra-layer connections, 28 and  $\frac{1}{2}$  and  $\frac{$ 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  $\frac{30}{30}$  induced graph can also be called a subHMN. An induced graph comes with all the types of nodes and  $\frac{30}{30}$ 31 31 node *u*, the function *connection* 2 takes three induced graphs  $G_{ii}$ ,  $G_{jj}$  and  $G_{ij}$  where  $i = l$  and  $j \in L \setminus l$ .  $\frac{33}{24}$  assigned to the layer 1. In making a cross-layer connection with layer 2, if there are sufficient nodes 34 34  $(35 \times m_{12})$  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<br>created once there are sufficient nodes in layer 2 created once there are sufficient nodes in layer 2.  $37 \times 37$ edges associated with vertex set  $V_i$  in layer *i* and  $V_j$  in layer *j*. For the inter-layer connections with the Let us consider a situation where no nodes are in the inter-layer subHMN  $G_{12}$  and a new node (*u*) is

<sup>38</sup> **Remark 5.1.** The above algorithm assigns a node to a single layer, making it incapable of generating a <sup>38</sup> <sup>39</sup> multiplex network without certain modifications.<sup>39</sup> multiplex network without certain modifications. 40 40

## 41 41 *5.2. Complexity Analysis and Scalability* 42 42

43 43 Adding a new node in layer *l* triggers two functions, *conn1* and *conn2*, for intra layer and inter layer <sup>44</sup> link generation. The algorithm establishes the intra layer links in  $O(m)$  time where  $m = M_{ll}$ . Here  $M_{ll}$  <sup>44</sup> <sup>45</sup> denotes the minimum number of connections a node makes in its layer. Following the intra layer links, <sup>45</sup> 46 46

<span id="page-10-0"></span><sup>1</sup> **Algorithm 1:** Generating an HMN 2  $\frac{1}{2}$  2  $\frac{1}{2}$  2  $\sum_{i=1}^{n} a_i$  $\frac{4}{4}$   $\frac{4}{4}$  $\frac{1}{2}$   $\frac{20}{20}$  and  $\frac{20}{20}$  finds to  $\frac{6}{20}$  $\frac{7}{7}$   $\frac{3}{7}$  with note  $\frac{27}{7}$  $\frac{1}{8}$   $\frac{1}{8}$   $\frac{1}{8}$   $\frac{1}{8}$   $\frac{1}{8}$  $\frac{9}{9}$  9  $\frac{1}{10}$   $\frac{1}{10}$  10 10  $\frac{11}{11}$  11  $\frac{11}{11}$  11 12 12 <sup>8</sup> *<sup>G</sup>ii* <sup>=</sup> *connection1*(*Gii*, *node*, *<sup>M</sup>ii*, α, β)  $\frac{13}{13}$   $\frac{13}{13}$   $\frac{13}{13}$  $\frac{14}{14}$  10  $\frac{14}{14}$  14 11  $G_{ij} = \text{connection2}(G_{ii}, G_{jj}, G_{ij}, \text{node}, M_{ij}, \alpha, \beta)$  $16 \t 12 \t node = node + 1;$ 17 <u>– Ferdinand States (</u>† 1788)<br>17 juli – Antonio States († 1798)<br>17 juli – Antonio States († 1798) **Input:** *N*, *L*, *R*<sub>*L*</sub>, *M*, α, *β* Output: Return HMN G 1 *node*  $\leftarrow$  1,  $R_{VI} \leftarrow \{\}$ 2  $G =$  *Empty HMN* 3 while  $node < N$  do<br>4  $i = uniformRa$  $i = uniformRandom(L)$  $\mathbf{s}$  |  $R_{VL}(node) = i$ 6  $t = uniformRandom(R<sub>L</sub>(i))$  $\begin{array}{c|c} \n7 & G_{ii}.addNode(node) \ \n8 & G_{ii} = connection1(\n\end{array}$ 9 while *j* ∈ *L* do 10 **if**  $i \neq j$  then

<sup>19</sup> we make inter layer connections for the node with all other layers in  $O(|L|m')$  considering the worst <sup>19</sup> 20 2009 where  $|I|$  denotes the number of levers and  $m' = \max(M)$ . It must be noted that the worst case  $20$ <sup>20</sup> case. where |*L*| denotes the number of layers and  $m' = \max_{j \in L} (M_{lj})$ . It must be noted that the worst case <sup>20</sup><sup>21</sup> <sup>22</sup> will arise when the node needs to connect to every other node in every layer. *j*∈*L*

#### $24$  24  $25$   $\bullet$  between a reason to the first  $\prime$ 6. Structural Measures of HMN

26 26  $\frac{27}{27}$  In this section, we define some of the structural measures of HMN. By definition HMN uses direction  $\frac{27}{27}$ for an edge  $e \in E$ . However, many network measures consider the in-links and out-links together. When  $\frac{28}{28}$ applicable, notations related to in-links and out-links are superscripted with *IN* and *OUT* respectively  $\frac{29}{29}$  $\frac{30}{30}$  and the following text. in the following text.

**31 Definition 6.1** (Out/In-Neighborhood in HMN). The Out/In-neighborhood of a node  $v^l$  is defined by the <sup>31</sup> <sup>32</sup> 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 <sup>32</sup>  $33$  a type  $t \in \mathcal{T}$ . That is,  $34$   $34$ 

$$
N^{IN}(v^l, \mathcal{L}, \mathcal{T}) = \{u^k | (u^k, v^l) \in E, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\}\
$$
  
\n
$$
N^{OUT}(v^l, \mathcal{L}, \mathcal{T}) = \{u^k | (v^l, u^k) \in E, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\}\
$$
  
\n
$$
37
$$
  
\n
$$
38
$$
  
\n(5) 37  
\n38

**Remark 6.1.** The definition of neighborhood is flexible to include as many types of nodes and layers 40 **Exercise 2021** and the community of the ground of the contract of method as many systems and movement of the contract of t we wish to take. To get all types of neighbors in all the layers we set  $\tau = T_V$  and  $\epsilon = L$  where  $T_V$  and  $L_{42}$   $L$  denote all vertices and layers respectively.

<sup>43</sup> **Remark 6.2.** A node can be present in more than one layers. One should note that the definition of <sup>43</sup>  $44$  neighborhood presented here does not contain the neighbors that the same node *v* in layer *k* may have  $44$  $\frac{45}{45}$  where  $k \neq l$   $\frac{45}{45}$ 46 46 where  $k \neq l$ .



<span id="page-11-0"></span>

<span id="page-12-2"></span><span id="page-12-0"></span>**Definition 6.2** (Neighborhood in HMN). The neighborhood of a node  $v^l$  is defined by  $N(v^l, \mathcal{L}, \mathcal{T}) =$ <br>  $N^{lN}(v^l, \mathcal{L}, \mathcal{T}) + N^{OUT}(v^l, \mathcal{L}, \mathcal{T})$  $N^{IN}(\nu^l, \mathcal{L}, \mathcal{T}) \cup N^{OUT}(\nu^l, \mathcal{L}, \mathcal{T}).$  $3$   $3$ **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  $T$  and belonging to a layer in 6 6 L to the count of all nodes of type in T and any layer in L. That is, 7 7 8 access to the contract of th 9  $|N(v^l \cap T)|$ <sup>9</sup><br>
10  $DC(v^l, \mathcal{L}, \mathcal{T}) = \frac{|N(v^l, \mathcal{L}, \mathcal{T})|}{|\{u^k|k \in \mathcal{L}, u \in V, u^k \neq v^l, R_{VT}(u) \in \mathcal{T}\}|}$  (6) <sup>9</sup><br>
11  $11$   $11$ 12 **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 12 <sup>13</sup> 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 <sup>13</sup> <sup>14</sup> case of a unweighted HMN the weights of all edges are 1) of the edges in the path is minimized. There <sup>14</sup> <sup>15</sup> can be more than one shortest path between two nodes and the set of all such shortest paths is denoted<sup>15</sup> <sup>16</sup> 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  $v^l$  <sup>16</sup> and  $w^k$ . When there is no path between  $v^l$  and  $w^k$  the  $d(v^l, w^k)$  is  $\infty$ .<br>18  $18$  18 19 **Definition 6.5** (HMN Betweeness Centrality). Given  $\mathcal L$  and  $\mathcal T$  the betweeness centrality of a node  $v^l$  in 19 20 a heterogeneous multi-layered network is the fraction of shortest paths between any two nodes  $x^k$  and  $y^j$  20 21 (where  $R_{VT}(x)$ ,  $R_{VT}(y)$  ∈  $\mathcal{T}$ ,  $k$ ,  $j$  ∈  $\mathcal{L}$ ) passing through node  $v^l$  among all the shortest paths between  $x^k$  21 22 and y<sup>j</sup>. If there is no path between  $x^k$  and y<sup>j</sup> then  $\frac{[\mathfrak{sp}(x^2, y^2 | y^2)]}{\mathfrak{p}}$  is considered to be 0. That is. 23 23 24 24 25  $\sim$  25 26  $BC(v^l, \mathcal{L}, \mathcal{T}) = \sum_{l} \frac{|\mathcal{P}(\mathcal{L}, v, \mathcal{T}^l|V^l)|}{2}$ 27  $x^k, y^j \in V'$   $|P(P(x^k, y^j)|)$  (7) 27 28 28 where *V* ′ = {*u i* <sup>|</sup>*<sup>i</sup>* ∈ L, *<sup>R</sup>VT* (*u*) ∈ T , *<sup>u</sup>* <sup>∈</sup> *<sup>V</sup>*, *<sup>u</sup> i* ̸= *v l* } 29  $\frac{1}{2}$  29 <sup>30</sup> If we are considering only cross layered connections then we can set the *layers* variable to  $L - R_{VL}(v^l)$ .  $31$   $\frac{1}{21}$   $\frac{1}{31}$   $\frac{1}{31}$  $\frac{32}{32}$  The cross layered betweeness will indicate the importance of a node outside its own layer. **33 Definition 6.6** (HMN Closeness Centrality). Given  $\mathcal L$  and  $\mathcal T$  the closeness centrality of a node  $v^l$  in a <sup>33</sup>  $34$  heterogeneous multi-layered network is the average shortest path length from  $v<sup>l</sup>$  to all other nodes of a  $34$ <sup>35</sup> and type in  $\tau$  in the network.<sup>35</sup>  $36$ 37 37 and *y*<sup>*j*</sup>. If there is no path between  $x^k$  and  $y^j$  then  $\frac{|sp(x^k, y^j|y^j)|}{|sp(x^k, y^j)|}$  $\frac{sp(x^x, y^y | V)}{|sp(x^k, y^j)|}$  is considered to be 0. That is,  $BC(v^l, \mathcal{L}, \mathcal{T}) = \sum_{x^k, y^j \in V'}$  $\frac{|sp(x^k, y^j | v^l)|}{|sp(x^k, y^j)|}$  $|sp(x^k, y^j)|$ (7)

<span id="page-12-4"></span><span id="page-12-3"></span>

38 38 39 39 40 40 *CC*(*v l* , <sup>L</sup>, <sup>T</sup> ) = <sup>X</sup> *u k*∈*V*′ 1 *d*(*v l* , *u k*) (8)

41 where  $V' = \{u^k | u \in V, u^k \neq v^l, k \in \mathcal{L}, R_{VT}(u) \in \mathcal{T}\}\$ <br>42 42

<span id="page-12-1"></span>**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*<br>44 *A homogeneous network* (*Lemma 4.3*) the neighborhood of a node  $v^l \in V$  is equivalent to the neighbor- $44$  a homogeneous network (Lemma [4.3\)](#page-6-1), the neighborhood of a node  $v^l \in V$  is equivalent to the neighbor-45 45 *hood of v in a homogeneous network.*46 46

<span id="page-13-0"></span>1 **Proof.** Given HMN *G* is nothing but a homogeneous network as per Lemma [4.3.](#page-6-1) The Definition [6.2](#page-12-0) 1 considers all types of neighbors of a node  $v^l$  in all the layers when  $|L| = 1$ ,  $T_V$ ,  $T_E = {\perp}$  which is a nothing but the degree of the node  $v^1$ ; making the neighborhood of HMN equivalent to the neighborhood 3 nothing but the degree of the node  $v^1$ ; making the neighborhood of HMN equivalent to the neighborhood  $\overline{3}$ 4 of the homogeneous network (Definition [2.2\)](#page-2-0) it represents. □ 5 5 6 **Corollary 6.1.1.** *Given an HMN which is a homogeneous network (Lemma [6.1\)](#page-12-1),*  $DC(v^l, \mathcal{L}, \mathcal{T})$  *6 6<br><i>Equation 6)* =  $DC(v)$  (*Equation 9*)  $7$  *(Equation [6](#page-12-2))*  $\equiv DC(v)$  *(Equation [2](#page-2-1))*. 8 access to the contract of th <sup>9</sup> **Proof.** The neighborhood of an HMN with parameters according to Lemma [6.1](#page-12-1) is equivalent to the  $_{10}$  neighborhood of a homogeneous network. Thus, the numerator in Equation [6](#page-12-2) is equivalent to the number  $_{10}$  $_{11}$  of neighbors of a node (making numerator in Equation [6](#page-12-2) = Equation [2\)](#page-2-1). The denominator in Equation  $_{11}$  $_{12}$  [6](#page-12-2) contains all the nodes of the network (an HMN equivalent to a homogeneous network) except  $v^l$  (the  $_{12}$ 13 node whose centrality we are trying to find). So, the denominator in Equation [6](#page-12-2) is equivalent to the 13 denominator in Equation [2.](#page-2-1) Thus, it is proved that  $DC(v^l, \mathcal{L}, \mathcal{T}) \equiv DC(v)$ . □ 15 15 **Corollary 6.1.2.** The shortest path between two nodes of an HMN with parameters  $|L| = 1, T_V, T_E = 16$ <br> $I \cup$  is equivalent to the shortest path between the same nodes in a homogeneous network  $_{17}$   $\{\perp\}$  *is equivalent to the shortest path between the same nodes in a homogeneous network.*  $18$  18 **Proof.** When we have only a single layer, i.e.,  $|L| = 1$  and a single type of vertex and edge, i.e.,  $\frac{19}{2}$  $T_V$ ,  $T_E = {\perp}$  then we consider nodes belonging to all the layers and node types in the shortest path by  $T_{20}$ <br>default (as an HMN is a homogeneous network with the given parameters as per Lemma 4.3) making  $_{21}$  default (as an HMN is a homogeneous network with the given parameters as per Lemma [4.3\)](#page-6-1) making  $_{21}$ 2<sup>1</sup> the shortest path in an HMN equivalent to the shortest path in a homogeneous network.  $\Box$  $23$ **Corollary 6.1.3.** *Given an HMN which is a homogeneous network (Lemma [6.1\)](#page-12-1),*  $BC(v^l, \mathcal{L}, \mathcal{T})$  $24$  $24$  $25$  *(Equation [7](#page-12-3))*  $\equiv BC(v)$  *(Equation [3](#page-2-2))*. 26 <u>- Johann Stein, american provincial provin</u> **Proof.** The shortest path between two nodes of an HMN with parameters as in Corollary [6.1.2](#page-13-0) is equiv-28 alent to the shortest path between the same nodes of a homogeneous network. Thus the numerator and 28  $\frac{28}{29}$  denominator in Equation [7](#page-12-3) is equivalent to the numerator and denominator in Equation [3.](#page-2-2) □ 30 30 **Corollary 6.1.4.** *Given an HMN which is a homogeneous network (Lemma [6.1\)](#page-12-1)*,  $CC(v^l, \mathcal{L}, \mathcal{T})$  <sup>31</sup><sup>31</sup>  $\sum_{32}^{32}$  *(Equation [8\)](#page-12-4)*  $\equiv CC(v)$  *(Equation [4](#page-2-3))* . **Proof.** The Distance between two nodes of an HMN with parameters as in Corollary [6.1.2](#page-13-0) is equivalent  $\frac{33}{24}$  $34$  to the distance between the same nodes of a homogeneous network. Thus the numerator and denominator  $34$ 35 . In the distribution of the same news of a nonlingence of news in the case in a manipulate and distribution  $\frac{35}{36}$  in Equation [8](#page-12-4) is equivalent to the numerator and denominator in Equation [4.](#page-2-3)  $\Box$ 37 37 38 38 **Definition 6.7** (HMN Clustering Co-efficient). Given  $\mathcal L$  and  $\mathcal T$ , the clustering coefficient (CCo) of a <sup>39</sup>  $^{40}$  node,  $v^l$ , in a heterogeneous multi-layered network is defined as the fraction of triangles that the node  $v^l$   $^{40}$ <sup>41</sup> participates in, out of the total number of triangles possible through that node. That is, <sup>41</sup> 42 42 43  $2 * |Triangle(s(x^k, y^j, y^l))|$  43 *CCo*( $v^l$ ,  $\mathcal{L}$ ,  $\mathcal{T}$ ) =  $\frac{2 * |Triangles(x^k, y^j, v^l)|}{|N(v^l, \mathcal{L}, \mathcal{T})| * (|N(v^l, \mathcal{L}, \mathcal{T})| - 1)}$  (9) 44 45<br>
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46<br>
47, *R*<sub>VT</sub> (*x*<sup>*k*</sup>)  $\in \mathcal{T}$ , *R*<sub>VT</sub> (*y*<sup>*j*</sup>)  $\in \mathcal{T}$ <br>
46  $46$  46  $|N(v^l, \mathcal{L}, \mathcal{T})| * (|N(v^l, \mathcal{L}, \mathcal{T})| - 1)$ (9)

<span id="page-14-2"></span><span id="page-14-1"></span>

<sup>21</sup> We can prove all the Lemmas and Corollary for clustering co-efficient in a similar manner as shown in <sup>21</sup>  $\frac{22}{2}$  the previous definitions. 23  $\frac{1}{2}$  23

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 $20$   $20$ 

## <span id="page-14-0"></span>26 26 7. Experiment and Results

<sup>28</sup> Experiments have been performed to show the ability of the proposed algorithm to generate heteroge-<sup>28</sup> <sup>29</sup> neous multilayered networks with structural properties close to real-world networks. We try to generate <sup>29</sup> 30 30 a Twitter network and an European air transportation network by changing certain parameters of our al-<sup>31</sup> gorithm. Further experiments are performed to compare the degree distributions and centrality measures<sup>31</sup> <sup>32</sup> of the generated synthetic network with their real counterparts. We report only the degree distribution <sup>32</sup> 33 of the nodes of both the real and synthetic network in the case of a large graph like Twitter. For the <sup>33</sup> <sup>34</sup> smaller air transportation network we present a comparison of the degree distributions along with other <sup>34</sup> <sup>35</sup> structural properties like centrality measures and clustering co-efficients. In both the cases we include<sup>35</sup> 36 36 comparisons with existing generation algorithms.

<sup>37</sup> It must be noted that we generated an HMN with two layers for representing the real Twitter network<sup>37</sup> <sup>38</sup> with parameter values  $L = \{1, 2\}$ ,  $R_L(1) = R_L(2) = \{t_1, t_2\}$ . The HMN for modelling air transportation<sup>38</sup><br><sup>39</sup> was generated using parameter values  $I = \{1, 2, 3, 4\}$ .  $R_L(i) = \{t_1\}$ . We can also generate homo-<sup>39</sup> was generated using parameter values  $L = \{1, 2, ..., 37\}$ ,  $R_L(i) = \{t_1\}$ . We can also generate homo-<br><sup>40</sup> generate heterogeneous as well as multilayered networks using our proposed algorithm. In order to <sup>40</sup> <sup>40</sup> geneous, heterogeneous as well as multilayered networks using our proposed algorithm. In order to <sup>40</sup> <sup>41</sup> generate homogeneous networks we can set the values of  $L = \{1\}$  and  $R_L(1) = \{t_1\}$ . The heteroge-<sup>41</sup> <sup>42</sup> neous networks can be generated with  $L = \{1\}$ ,  $R_L(1) = \{t_1, t_2, ..., t_k\}$  and multi-layered networks can  $\frac{42}{1}$ <br><sup>43</sup> be generated with  $I = \{1, 2, 3, ..., k\}$   $R_L(i) = \{t_1\}$  parameters. The *m* values for all the networ <sup>43</sup> be generated with  $L = \{1, 2, 3, ..., k\}$ ,  $R_L(i) = \{t_1\}$  parameters. The *m* values for all the networks are <sup>43</sup> nositive samples generated from a normal distribution with a mean of 2 and a standard deviation of 1 <sup>44</sup> positive samples generated from a normal distribution with a mean of 2 and a standard deviation of 1. <sup>44</sup> <sup>45</sup> The use of *m* values in this range generated degree distributions with a scale free property.

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<span id="page-15-0"></span>16 *Chatterjee and Kundu / HMN*

$\sim$ Table 4	



<span id="page-15-1"></span>

10 **Comparison of Generated network with Miscellaneous networks** 10



#### 25 and  $\sim$  25  $26$   $\ldots$   $\ldots$   $26$   $\ldots$   $26$ *7.1. A real world dataset*

<sup>27</sup> 27 We have used a Twitter dataset [\[40\]](#page-20-15) (referred to here as *TWITT*) and represented it in the format as  $\frac{27}{20}$ 28 shown in Figure [2.](#page-7-0) A tweet can be easily classified as aggressive or non-aggressive based on a standard  $\frac{29}{28}$  language classification model. The Twitter network has 20125 nodes and 3938046 edges in the tweet 30 30 layer (layer 1), 35936 nodes and 60824 edges in the user layer (layer 2) and 93123 edges in the user-<br>31  $32$   $32$   $32$ tweet layer (interlayer connection).

## 33 33 *7.2. Modelling TWITT with existing generation models*  $34$   $34$

<sup>35</sup> In our literature survey we have not found existing methods for generating a generic heterogeneous or <sup>35</sup> <sup>36</sup> a multi-layered network so we compare the structural properties of the HMN generated by Algorithms<sup>36</sup> <sup>37</sup> [1](#page-10-0) and [2](#page-11-0) with the existing homogeneous models. The homogeneous models used are the Barabasi-Albert<sup>37</sup> <sup>38</sup> (BA) model [\[3\]](#page-18-0), Erdos-Reyni (ER) model [\[33\]](#page-20-16), Internet as graph [\[32\]](#page-20-17), Gnm random graph. In each of the <sup>38</sup> <sup>39</sup> Figures [5a, 5b, 5c,](#page-16-0) we have compared the degree distribution of the largest component of different layers<sup>39</sup> <sup>40</sup> of the TWITT network with graphs generated from the aforementioned models as well as proposed<sup>40</sup> <sup>41</sup> synthetic network. Each of the generated graphs have comparable nodes and/or edges.<sup>41</sup>

<sup>42</sup> As we can see from the Figures [5a, 5b](#page-16-0) and [5c](#page-16-0) our proposed HMN (referred to using the keyword <sup>42</sup> <sup>43</sup> synthetic) is very close to the degree distribution of the actual TWITT dataset except for the user-tweet<sup>43</sup> <sup>44</sup> layer. It must be noted our proposed network does not have any node having a degree less than the <sup>44</sup> <sup>45</sup> thresholds defined in *M*, similar to a BA network. When we compare our results with other models we <sup>45</sup> 46 46

<span id="page-16-0"></span>

12 12 Fig. 5. Comparing the smoothed degree distribution of the different layers of the TWITT network with our synthetic network 13 and state stational decreases on a regularization of the state. and other standard networks on a logarithmic scale.

 $11$   $11$ 

<sup>14</sup> see that our model is consistent across the layers which shed light on the generic nature of our model. <sup>14</sup> <sup>15</sup> We have considered the interlayer as well as the intralayer degree of a node for preferential attachment, <sup>15</sup> <sup>16</sup> and from the Figures [5a](#page-16-0) - [5c](#page-16-0) it is evident that it well describes a real-world network.<sup>16</sup>  $17$  and  $17$  and  $17$  and  $17$  and  $17$  and  $17$ 

## 18 18 *7.3. Generating existing networks*  $19$  19

<sup>20</sup> We have successfully shown the generation capabilities of HMN for generating large heterogeneous <sup>20</sup>  $21$  networks with more than 10000 nodes. To demonstrate the capabilities of HMN for generating smaller  $21$ <sup>22</sup> networks we have tried to model the smaller European air transportation network [\[15\]](#page-19-9) abbreviated as  $22$ <sup>23</sup> *EATN*. The air transportation network is also a multiplex network having 37 different layers with each <sup>23</sup> <sup>24</sup> one of the layer representing a different airlines of Europe. To compare our results with existing models <sup>24</sup> <sup>25</sup> we have taken the BINBALL [\[5\]](#page-19-14) generative model designed especially for modelling the multiplex  $25$ <sup>26</sup> air transportation network. We have generated 10 layers of the air transportation network using both<sup>26</sup> <sup>27</sup> BINBALL and HMN and compared the average centrality measures of the air transportation network<sup>27</sup> <sup>28</sup> with both the generated networks. The results are shown in Table [2.](#page-14-1) It must be noted that the results  $28$ <sup>29</sup> presented in Table [2](#page-14-1) are averaged over the nodes of each of the layers in the multiplex network. The <sup>29</sup> <sup>30</sup> column Triangles/node denotes the average number of triangles any node participates in averaged over <sup>30</sup> <sup>31</sup> all the layers. In addition to the centrality measures, we compare the degree distribution of 2 layers<sup>31</sup> <sup>32</sup> sampled randomly from the EATN with randomly sampled layers generated from BINBALL and HMN <sup>32</sup> <sup>33</sup> as shown in Figure [6](#page-18-1) (our proposed network is referred to as HMNG).<sup>33</sup>

<sup>34</sup> The air transportation and Twitter networks alone do not represent the existing breadth of networks <sup>34</sup> <sup>35</sup> in the literature. To show the generalization capability of our proposed algorithm, we have tried to <sup>35</sup> <sup>36</sup> generate networks belonging to different domains like small molecule datasets (PTC-MR, PTC-FM), <sup>36</sup> <sup>37</sup> biological networks (bio-DM-HT, bio-grid-mouse, Bio-yeast-protein-inter), networks of nitroaromatic <sup>37</sup> <sup>38</sup> compounds (Mutag), crystal growth eigenmode graphs (cryg2500), combinatorial problems (bibd-15-3), <sup>38</sup> <sup>39</sup> computational fluid dynamics graph (Watt-2), linear programming problems (lpi-bgdbg1), eigenvalue<sup>39</sup> <sup>40</sup> model reduction problems (M80PI-n1, S80PI-n1), chemical datasets (ENZYMES-g272, g366, g392, <sup>40</sup> <sup>41</sup> g117, g526, g527, g349, g103, g295, g296), brain networks (bn-mouse-kasthuri-graph-v4) and even <sup>41</sup> <sup>42</sup> crime dataset (Ia-crime-moreno). We have collected the networks from [\[80\]](#page-22-0). Networks belonging to <sup>42</sup> <sup>43</sup> different domains have different structural properties such as degree, density, centrality measure, number<sup>43</sup> <sup>44</sup> of triangles and assortativity, etc. We have compared our generated network with the existing networks <sup>44</sup> <sup>45</sup> on such structural parameters. The results are shown in Table [3,](#page-14-2) [4,](#page-15-0) [5.](#page-15-1) We have considered other structural  $45$ 46 46 1 1 measures apart from centrality measures. This includes density, average degree, assortativity, triangle 2 2 counts, clustering co-efficient, and the number of max cliques. It must be noted that in all the tables, CC

3 3 denotes clustering co-efficient.

4 4 In our experiments, we have seen that a single graph generated from our algorithm with different 5 parameter values ( $\alpha$ , β and *M*) for different layers (both intra and inter) can model different networks 5<br>5 with varying intra-layer and inter-layer properties. This can be seen for the enzyme networks  $\alpha$ 103  $\alpha$ 6 6 with varying intra-layer and inter-layer properties. This can be seen for the enzyme networks *g*103, *g*295 7 7 and *g*296, which are modelled using different layers of the same graph using parameters as mentioned 8 8 in Table [3.](#page-14-2) The graph *g*103 is modelled using generated intra-layer graph whereas *g*295 and *g*296 are 9 9 modelled using inter-layer graph. It must be noted that the number of triangles in an inter-layer graph <sup>10</sup> is inherently zero. We combine the inter-layer graph with the edges of an intra-layer graph to model <sup>10</sup> 11 different network characteristics. Also, in Table [3,](#page-14-2) we observe that increasing the values of α and β 11<br>12 increases the number of triangles and the average degree for the networks generated using intra layers 12 <sup>12</sup> increases the number of triangles and the average degree for the networks generated using intra layers <sup>12</sup> 13 as shown in the first 4 sets of rows of Table [3.](#page-14-2) In the case of biological networks shown in Table [4](#page-15-0) with a 13 <sup>14</sup> comparable number of nodes, the average degree remains similar even for a small decrease in the value <sup>14</sup> 15 of β. We have found the average degree, assortativity and clustering coefficient to increase when alpha 15<br>16 and heta increase. The value of assortativity increases with alpha even when heta decreases but it takes a <sup>16</sup> and beta increase. The value of assortativity increases with alpha even when beta decreases, but it takes a <sup>17</sup> bigger jump when we increase alpha with beta. In the last row of Table [4,](#page-15-0) we have increased the value of <sup>17</sup> <sup>18</sup> the parameter *M* to analyze the structural similarity when the number of nodes is very similar. Increasing <sup>18</sup> <sup>19</sup> the value of *M* by 1 increases the number of edges keeping other aspects of the network comparable. In <sup>19</sup> <sup>20</sup> Table [5,](#page-15-1) we compare our results to different types of nodes that cannot be grouped under one category. <sup>20</sup> <sup>21</sup> We have achieved zero triangles in certain networks using inter-layer connections without intra-layer<sup>21</sup> <sup>22</sup> edges. It must be noted that there is a randomness in the selection of neighbours of a node which results<sup>22</sup> <sup>23</sup> in non-determinism, i.e. network properties may vary slightly even with the same parameter values. <sup>23</sup> 24 24

# $25$  25

## <span id="page-17-0"></span>26 26 8. Discussion and Conclusion

<sup>28</sup> In this paper, we introduced a new model Heterogeneous Multilayered Network (HMN), which is a <sup>28</sup> 29 29 generalized network model capable of representing any complex networks of type homogeneous, het-30 30 erogeneous, multilayer and their combinations. We also defined different structural measures on HMN. <sup>31</sup> We have proved that the set of all HMNs is a superset of the set of all homogeneous, heterogeneous, and <sup>31</sup> 32 32 multi-layered networks.

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<sup>33</sup> In addition, a parameterized algorithm is presented to generate an HMN synthetically. We show that <sup>33</sup> <sup>34</sup> the algorithm is able to generate a homogeneous, heterogeneous, and multilayered network by changing <sup>34</sup> <sup>35</sup> parameter values. Through experiments, we show that all networks generated by this algorithm have <sup>35</sup> 36 36 scale-free properties.

<sup>37</sup> The network generated by the algorithm is generalized and can be tweaked by changing the parameter <sup>37</sup> <sup>38</sup> values for applications in certain areas where networks largely follow a scale-free property. These syn-<br><sup>38</sup> <sup>39</sup> thetic networks will open the opportunity to research with HMNs that is otherwise difficult to conduct <sup>39</sup> <sup>40</sup> due to the unavailability of the data. Although heterogeneous network data are available, to the best of <sup>40</sup> <sup>41</sup> our knowledge, there is no algorithm for generating a heterogeneous network and the proposed algo-<sup>41</sup> <sup>42</sup> rithm would encourage research with heterogeneous networks as well. Note that the proposed algorithm <sup>42</sup>  $43$  can only be used to generate an undirected HMN. However, we believe that with minor changes, we can  $43$ <sup>44</sup> generate directed HMNs. To show the applicability of the generated networks using our proposed algo-<sup>44</sup> <sup>45</sup> rithm we have compared it to a real-world Twitter network as well as a multiplex EATN network. An  $45$ 46 46

<span id="page-18-1"></span>

 $^{26}$  Fig. 6. The figures compare the degree distributions of randomly selected layers from EATN with networks generated from  $^{26}$ 27 BINBALL and HMNG. 27

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<sup>29</sup> important future research is to show that our proposed definition of HMN holds for a dynamic network<sup>29</sup> 30 or a signed network.

<sup>31</sup> Finally, with this work, we tried to open a new avenue of research with complex networks. While <sup>31</sup> <sup>32</sup> the theories developed will help further theoretical analysis and provide the basis of application, the <sup>32</sup> <sup>33</sup> synthetic network generation algorithm will provide the opportunity to develop applications with HMN. <sup>33</sup>

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