

Symmetry based Structure Entropy of Complex Networks

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Precisely quantifying the heterogeneity or disorder of a network system is very important and desired in studies of behavior and function of the network system. Although many degree-based entropies have been proposed to measure the heterogeneity of real networks, heterogeneity implicated in the structure of networks can not be precisely quantified yet. Hence, we propose a new structure entropy based on automorphism partition to precisely quantify the structural heterogeneity of networks. Analysis of extreme cases shows that entropy based on automorphism partition can quantify the structural heterogeneity of networks more precisely than degree-based entropies. We also summarized symmetry and heterogeneity statistics of many real networks, finding that real networks are indeed more heterogenous in the view of automorphism partition than what have been depicted under the measurement of degree-based entropies; and that structural heterogeneity is strongly negatively correlated to symmetry of real networks.

PACS numbers:

INTRODUCTION

In recent years, great efforts have been dedicated to the research on complex networks, due to the fact that many complex systems can be modeled as networks consisting of components as well as relations among these components. Previous studies primarily focus on finding various statistical properties of real networks, especially degree based statistics, such as degree distribution[1, 2], degree correlation[3, 4, 5], degree-based structure entropies[6, 7]. Studies of many significant properties of networks, such as heterogeneity[1], assortative mixing[8, 9] and self-similarity [10, 11], are based on these statistics.

Degree delivers to us the most important information about the number of interconnections of each individual component in the network. However, degree only provides us a view of complex networks in a shallow level, for the reason that vertex partition [30] based on degree is coarser than many finer vertex partitions in many networks, e.g., automorphism partition — a core concept in the symmetry of network. In other words, in some networks, vertex with the same degree would be further differentiated from each other, thus forming a finer partition. Consequently, a fascinating problem arises, what will complex network looks like if automorphism partition is employed instead of degree partition? Since degree-based statistics are the driving forces of many existing studies in complex networks. We believe that studies of complex network in the view of symmetry will open a brand new field leading us to deeper understanding about complex networks.

There is increasingly recognition that measuring heterogeneity of complex networks is very important in studies of behavior and function of complex networks. It has been shown in [2] that heterogeneity of degree is directly related to the robust-yet-fragile property of scale-free networks, i.e., robustness against random failures of vertices but vulnerability to target attacks. Furthermore, it has been found in [12] that the homogeneous networks are more synchronizable than heterogeneous ones, even though the average network distance is large.

However, existing heterogeneity measures [6, 7] of complex networks are all based on degree. Specifically, entropy in [6] is based on remaining degree [8, 9] distribution and entropy in [7] is based on degree distribution. In fact, degree-based measures of heterogeneity are only the precise quantification of degree heterogeneity of networks, not that of actual heterogeneity in the sense of structure of many networks. To some extent, degree heterogeneity of networks is only the approximations of structural heterogeneity of networks. For example, as shown in Example .1, in some networks, vertices with the same degree still can be differentiated from each other through measurement on some structural properties of individual vertex, such as the number of triangles passing through a vertex, the shortest path passing through a vertex(also know as betweenness [13]). Hence, heterogeneity measured by degree partition can not precisely describe the structural heterogeneity for all networks. Luckily, automorphism partition of the network

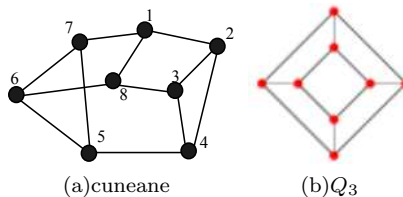


FIG. 1: Illustration of two 3-regular graphs. Figure (a) shows an abstract structure of molecule known as 'cuneane', which is not vertex transitive. Figure (b) shows an example of 3-cube graph, denoted as Q_3 , which is vertex transitive.

naturally partitions the vertex set into structurally equivalent cells, thus offering us an ideal alternative to measure the heterogeneity of network structure.

Example .1. As shown in Figure 1, 'cuneane' and Q_3 are all regular graphs with degree 3. Hence, structure of 'cuneane' and Q_3 can be considered as completely homogeneous if degree-based entropy measures are utilized. However, intuitively, we can see that homogeneity in 'cuneane' is different from that of Q_3 . All the vertices in Q_3 are equivalent from the structure perspective, thus forming a unit partition, and we can not further partition the vertex set. However, in 'cuneane', we can easily find that vertices 1 and 8 play a different role from that of vertices 4 and 5 or the remaining vertices, for the reason that 1 and 8 are the only ones not involved in the two triangles, 4 and 5 are the only ones connected by an edge between two different triangles. Therefore, for 'cuneane', we can construct a vertex partition $\mathcal{P} = \{\{1, 8\}, \{4, 5\}, \{2, 3, 6, 7\}\}$, which is finer than degree partition. Furthermore, we can validate that partition \mathcal{P} is just the automorphism partition of 'cuneane'.

SYMMETRY-BASED STRUCTURE ENTROPY

A graph is denoted as $G = G(V, E)$, where V is the set of vertices and $E \subseteq V \times V$ is the set of edges. If $(v_1, v_2) \in E$, then we say that v_1 and v_2 are adjacent. An automorphism acting on the vertex set can be viewed as a permutation of the nodes of the graph preserving the adjacency of the vertices. The set of automorphisms under the product of permutation forms a group[14]. In general, a network is *asymmetric* if its automorphism group is the identity group, which only contains a identity permutation; otherwise, the network is *symmetric*. A graph $G = G(V, E)$ is *vertex transitive*(or just transitive) if its automorphism group acts transitively on V , which means that for any two distinct vertices of V , there is an automorphism mapping one to the other.

Let $Aut(G)$ be the automorphism group acting on vertex set V . Then naturally, we can get a partition $\mathcal{P} = \{V_1, V_2, \dots, V_k\}$, called as automorphism partition, in the way that x is equivalent to y if and only if $\exists g \in Aut(G)$, s.t. $x^g = y$. And each cell of the partition is called as an orbit of the automorphism group $Aut(G)$. Automorphism partition offers us an in-depth insight into the heterogeneity of networks. Compared to the degree partition of the vertex set, automorphism partition is much finer than the degree partition for most of networks.

To accurately measure the structural heterogeneity of complex networks, we define an *entropy based on automorphism partition*, abbreviated as EAP, as follows:

$$EAP = - \sum_{1 \leq i \leq |\mathcal{P}|} p_i \log p_i \quad (1)$$

, where \mathcal{P} is the automorphism partition of the network, p_i is the probability that a vertex belongs to the cell V_i of \mathcal{P} . Note that given a network's automorphism partition $\mathcal{P} = \{V_1, V_2, \dots, V_k\}$, we can calculate p_i as:

$$p_i = \frac{|V_i|}{\sum_j |V_j|} = \frac{|V_i|}{N} \quad (2)$$

, where N is the number of vertices in a graph.

Obviously, the maximum value of EAP or EAP_{max} equals to $\log(N)$, obtained when $p_i = \frac{1}{N}$ for each $1 \leq i \leq |\mathcal{P}|$, i.e., the graph has a *discrete* automorphism partition. The minimum value of EAP or EAP_{min} equals to 0 and occurs when the automorphism partition is a *unit partition*, implying that all the vertex belong to the same cell or all vertex are equivalent in the structure of the network. The maximum value of EAP corresponds to the completely structure-heterogeneous network, i.e. asymmetric network, and the minimum value of EAP corresponds to the completely structure-homogeneous network, i.e. transitive networks(shown in Figure 3) .

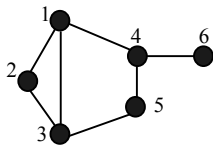


FIG. 2: Illustration of an asymmetric graph. The degree partition $\mathcal{D} = \{\{1, 3, 4\}, \{2, 5\}, \{6\}\}$ is much coarser than automorphism partition, which is a discrete partition in this graph. In the cell $\{1, 3, 4\}$ of degree partition, all vertices have degree 3, however, vertex 4 is the only one adjacent to a vertex with degree 1, which could distinguish vertex 4 from $\{1, 3, 4\}$. Vertex 1 is adjacent to two vertices with degree 3, while vertex 3 is only adjacent to one vertex with degree 3, which could differentiate vertex 1 from vertex 3. Hence, vertices 1, 3, 4 are not structure-equivalent to each other. Vertex 2 and 5 in the cell $\{2, 5\}$ of degree partition also can be differentiated from each other, because adjacent nodes of vertex 2 and adjacent nodes of vertex 5 are not structural equivalent, i.e. vertex 1 and vertex 4 are not structural equivalent.

The normalized entropy based on automorphism partition (NEAP) can be defined as:

$$NEAP = \frac{EAP - EAP_{min}}{EAP_{max} - EAP_{min}} = \frac{EAP}{\log N} \quad (3)$$

, where N is the number of vertices in the network.

For comparison, we denote entropy based on remaining degree distribution by ERDD [6] and entropy based on degree distribution by EDD [7]. We also define their corresponding normalized entropy similar to Equation 3, which are denoted by NERDD and NEDD respectively. Example .2 illustrates the computation of these three entropies.

Example .2. As shown in Figure 1, since 'cuneane' is a regular graph, we have $EDD = ERDD = NEDD = NERDD = 0$. However, the automorphism partition of 'cuneane' is not a unit partition, and we have $p_1 = p_2 = \frac{1}{4}$, $p_3 = \frac{1}{2}$. Thus $EAP = -\frac{1}{4} \log \frac{1}{4} - \frac{1}{4} \log \frac{1}{4} - \frac{1}{2} \log \frac{1}{2} = \frac{1}{2} \log 8$, $NEAP = \frac{\frac{1}{2} \log 8}{\log 8} = 0.5$, which is a value larger than 0, thus could quantify 'cuneane' as heterogenous in a certain degree rather than completely homogenous. Hence, in this case, EAP is more appropriate for quantifying structure-heterogeneity than ERDD and EDD.

The maximum values of ERDD or EDD are both $\log(N)$, however, the maximal values of two entropies correspond to two different kinds of networks, respectively. For EDD, the maximal entropy value corresponds to the completely degree-heterogenous networks, i.e., networks with N nodes partitioned into N non-empty cells. For ERDD, the maximal entropy value corresponds to the completely remaining-degree-heterogenous networks, i.e., networks with remaining degree equally distributed.

Completely degree-heterogenous networks are the most heterogenous cases under entropy measure of EDD. However, as shown in Figure 2, completely structure-heterogenous networks are not necessarily completely degree-heterogenous, note that the inverse statement necessarily holds true. As long as a network is asymmetric, i.e., the automorphism group contains no non-trivial permutations, the network structure will be completely heterogenous. Hence, extreme heterogenous cases should be extended to asymmetric networks provided that more precise evaluation of structural heterogeneity is desired (shown in Figure 3).

The minimum values of ERDD and EDD both equal to 0, both corresponding to regular networks, which are the most homogeneous networks under these two entropy measures. However, as shown in Example 1, regular graphs can be subdivided into transitive and non-transitive graphs, and only transitive graphs are the extreme structure homogeneous networks. Hence, extreme homogeneous cases should be limited to transitive networks if more precise evaluating of structural heterogeneity is desired (shown in Figure 3).

According to the above facts, the relation between degree-based entropies and symmetry based entropy also can be stated as following statements:

1. $f_{EDD}(G) = EDD_{max} \Rightarrow f_{EAP}(G) = EAP_{max}$, however, it does not necessarily hold true vice versa;
2. $f_{EAP}(G) = EAP_{min} \Rightarrow f_{EDD}(G) = EDD_{min}$, however, it does not necessarily hold true vice versa;
3. $f_{EDD}(G) = EDD_{min} \Leftrightarrow f_{ERDD}(G) = ERDD_{min}$;

where f_{EDD} , f_{ERDD} and f_{EAP} are the functions obtaining EDD, ERDD and EAP for each graph, respectively.

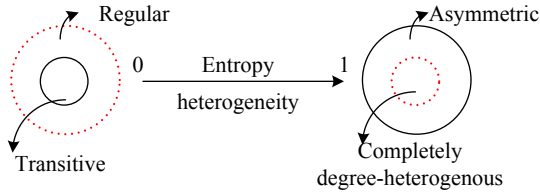


FIG. 3: Illustration of extreme cases under different entropy measures. The dotted circles represent the two extreme cases of NEDD. The solid circles represent the two extreme cases of NEAP. The embedding relation between circles express the containment relation between network set. Note that, the minimal cases of NERDD also can be represented by the left dotted circle, while the maximal case of NERDD should lie in the middle range of $[0,1]$ in terms of the measurement of NEDD or NEAP.

TABLE I: Statistics of some real networks and theoretic networks. Summarized statistics include some basic information about the network (All the networks are preprocessed as an undirected, unweighted graphs without any self-loops and multi-edges) including the number of the nodes N , the number of the edges M , the average degree z . The key measures quantifying symmetry of the network are also summarized, including the automorphism group size of the real networks α_G [15] (to simplify the representation, we use $\lg \alpha_G$); the ratio of α_G to the maximal automorphism group size of graphs with N nodes, defined as $\beta_G = (\alpha_G/N!)^{1/N}$ [16, 17]; the ratio of number of nodes in the non-trivial orbits to N , defined as $\gamma_G = \frac{\sum_{1 \leq i \leq k, |V_i| > 1} |V_i|}{N}$ [18]. We also generate four BA [1] networks with m (the number of nodes that a new node attach to) varying from 1 to 4 in increment of 1. And we generate four ER [19] networks with average degree approximately as one of $\{2,4,6,8\}$, using PAJEK [20].

Network	N	M	z	$\lg \alpha_G$	β_G	$\gamma_G(\%)$	NEDD	NERDD	NEAP
Technique Network									
USPowerGrid[21]	4942	6594	2.67	152.71	5.90×10^{-4}	16.7	0.20	0.25	0.98
InternetAS ^a	22443	45550	4.06	11346	3.8784×10^{-4}	76.1	0.16	0.39	0.84
Social Network									
arXiv ^b	27771	352285	25.37	333.26	1.01×10^{-4}	3.51	0.41	0.51	0.99
USAir97[24]	332	2126	12.81	24.41	9.59×10^{-3}	26.20	0.539	0.68	0.95
PairsP[25]	10617	63782	12.02	632.80	2.90×10^{-4}	24.32	0.32	0.47	0.97
foldoc[26]	13356	91471	13.6974	17	2×10^{-4}	0.80	0.32	0.39	1
Erdos02[27]	6927	11850	3.42	4222.5	1.6×10^{-3}	73.75	0.15	0.44	0.77
Biological Network									
BioGrid-SAC[28]	5438	73054	13.43	57.79	5.12×10^{-4}	3.2739	0.48	0.61	1.00
BioGrid-MUS[28]	219	400	3.65	126.93	4.69×10^{-2}	77.98	0.28	0.47	0.64
BioGrid-HOM[28]	7523	20029	5.32	935.09	4.81×10^{-4}	24.47	0.28	0.43	0.94
BioGrid-DRO[28]	7529	25196	6.69	624.32	4.27×10^{-4}	21.36	0.30	0.45	0.96
BioGrid-CAE[28]	2781	4350	3.13	829.69	1.94×10^{-3}	51.08	0.21	0.411	0.85
ppi[29]	1870	2203	4.7123	518.6	2.7×10^{-3}	53.32	0.21	0.34	0.82
Theoretic Networks									
Star Graph	2000	1999	1.99	5732.2	0.9962	99.95	5.65×10^{-4}	0.09	5.65×10^{-4}
BA(1)	2010	2000	1.99	282.09	1.90×10^{-3}	56.37	0.17	0.30	0.91
BA(2)	2010	4000	3.98	0.60	1.40×10^{-3}	0.2	0.24	0.35	1
BA(3)	2010	6000	5.97	0	1.35×10^{-3}	0	0.28	0.39	1
BA(4)	2010	8000	7.96	0	1.35×10^{-3}	0	0.31	0.43	1
ER(1)	2000	2081	2.08	507.97	2.4×10^{-3}	34	0.225	0.228	0.89
ER(2)	2000	4002	4	51.33	1.4×10^{-3}	2.65	0.276	0.274	0.99
ER(3)	2000	5923	5.90	2.07	1.36×10^{-3}	0.25	0.30	0.30	1
ER(4)	2000	8137	8.14	0	1.36×10^{-3}	0	0.32	0.32	1

^aHere, the snapshot at 2006-07-10 of CAIDA [22] is used

^bHere, the snapshot at 2003-04 of HEPCTH (high energy physics theory) citation graph [23] is used

ANALYSIS

In this section, we first show that in the view of symmetry, or automorphism partition, most of real networks should be characterized as more heterogenous than what have been shown in the view of degree partition. To show this, we calculated NEDD, NERDD and NEAP for 125 real networks. As shown in Figure 4, NEDD values of real networks tend to lie in the range $[0.2,0.8]$ (overall 87.2% networks lie in this range) and its mean value is 0.47; NERDD values

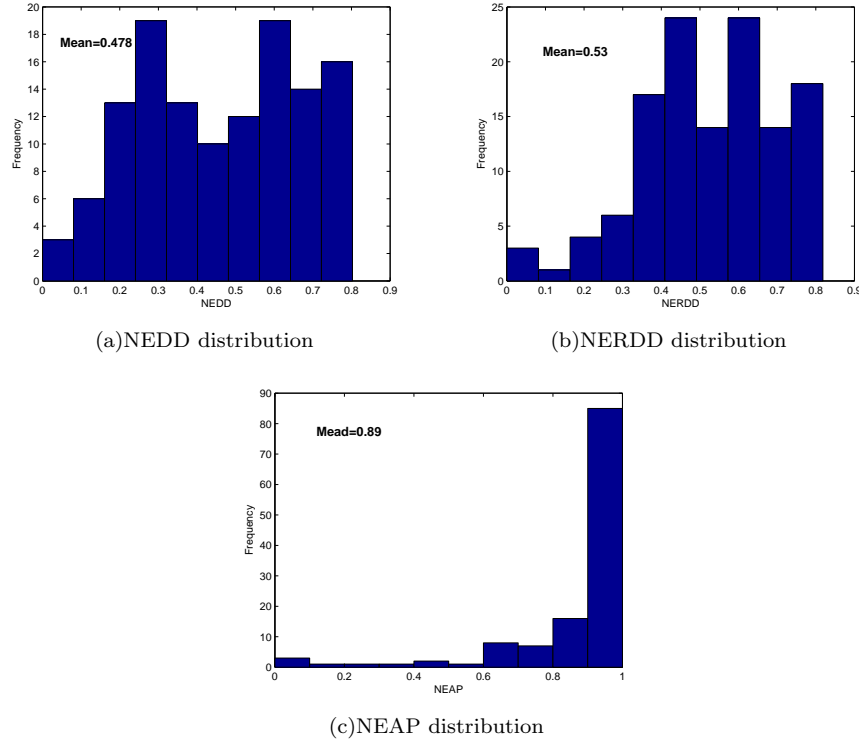


FIG. 4: Distribution of values of three entropy measures, NEDD, NERDD and NEAP for 125 real networks.

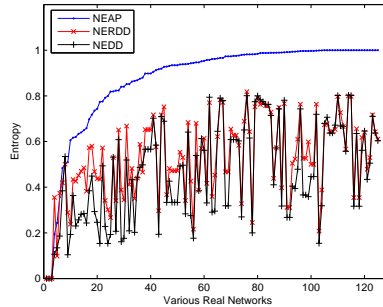


FIG. 5: Comparison of three entropy measures. The horizontal axis represent various networks in the ascending order of corresponding NEAP values.

of real networks tend to lie in the range $[0.4, 0.8]$ (overall 75.2% real networks lie in this range) and its mean value is 0.53; while NEAP of real networks primarily lies in the range $[0.8, 1]$ (overall 80.8% real networks lie in this range) and its mean value is 0.89, close to 1. In addition, for almost all the tested real networks, the value of NEAP is larger than that of NEDD and NERDD, which is shown in Figure 5. Hence, from these observations, we can see that real networks are very heterogeneous in the view of automorphism partition, and real networks will have a larger probability (larger than 80% in our samples) to be quantified with a NEAP value larger than 0.8.

We also need to note that some real networks characterized as very homogenous in the view of degree partition have been quantified as very heterogenous in the view of symmetry. As shown in Table I, for almost all the real networks, the corresponding values of the degree-based entropies are less than 0.5, except for the NERDD of arXiv, USAir97, BioGrid-SAC, and NEDD of USAir97; while for all the networks, the corresponding values of NEAP are larger than 0.6 and most of them larger than 0.8. If the median value of range $[0, 1]$ is taken as the critical value indicating whether a network is heterogenous, then many real networks under the measure of degree based entropies, are all tend to be quantified as homogenous. On the contrary, real networks under the measure of symmetry-based entropy tend to be quantified as very heterogenous.

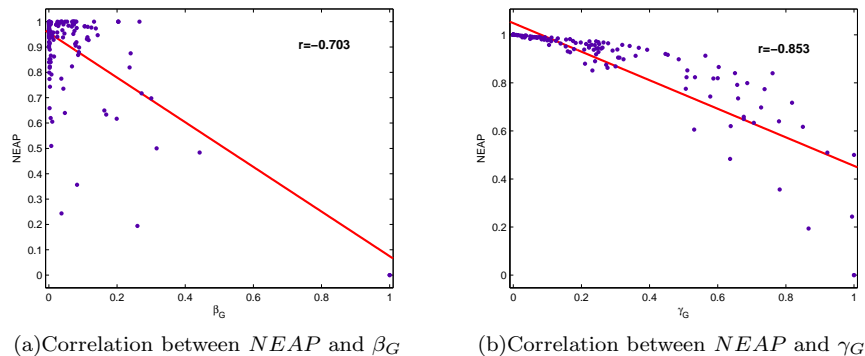


FIG. 6: . $NEAP$ appears to be negatively correlated to β_G and γ_G , and corresponding correlation coefficients are -0.703 and -0.853, respectively. 125 Real networks and 28 theoretic networks, overall 153 samples, are used.

Since heterogeneity based on automorphism partition describes the structure heterogeneity more accurately than degree-based heterogeneity, it's reasonable to believe that most of real networks are very heterogenous in their structure.

In Table I, statistics of some theoretic networks are also summarized. We can see that $NEAP$ of star graph is close to 0, indicating that star graph is very homogenous. Indeed, in a star graph, almost all nodes except for the central node lie in same cell of automorphism partition and these nodes can not be differentiated from each other by any means, thus it's natural that star graph is very homogenous.

Generally, scale free networks are considered to be more heterogenous than ER random networks [1], which is based on the intuitive observation that scale free networks are right-skewed in double-log degree distribution while the degrees of ER random networks are exponentially distributed with an obvious scale. However, no quantification or theoretic proof has been provided to verify the above notion, which can be partly attributed to the lack of appropriate measures of heterogeneity of real networks. However, utilizing three entropy measures, we can clearly see that under the measurement of $NEDD$ and $NERDD$, the difference of heterogeneity between scale free and random networks are very small (less than 0.05), and under the measure of $NEAP$, both scale free and random networks tend to be quantified as very heterogenous without clear difference (less than 0.02).

Next, we will show that structural heterogeneity is strongly negatively correlated to the symmetry of networks, which means that the less symmetric a network is, the more structure-heterogenous the networks is. As shown in Figure 6, strong negative relation could be observed from the $\beta_G - NEAP$ and $\gamma_G - NEAP$ correlation curves. In fact, if a network is very symmetric, nodes of the graph will have higher probability to be equivalent in the structure, thus the automorphism partition will be much closer to a *unit partition*, which is extremely homogenous. Conversely, if the network is closer to a asymmetric network, vertex can be easily differentiated from each other from the structural perspective, leading to a nearly discrete automorphism partition. Consequently, the whole network tends to be structure-heterogenous.

CONCLUSION

We have shown that entropies based on degree partition can not precisely describe the structural heterogeneity of complex networks in many cases due to its inability to differentiate vertices with the same degree. Instead, due to the strength of automorphism partition that can naturally partition vertex set into equivalent cells from the structure perspective, entropy based on automorphism partition can quantify the heterogeneity of networks more accurately.

Networks with extreme heterogeneity and homogeneity under different entropy measures, including two degree-based entropy and symmetry based entropy, have been analyzed, showing that symmetry-based entropy is more accurate in quantifying the heterogeneity or disorder of a network system than degree-based entropies. We also calculated symmetry and heterogeneity statistics for hundreds of real networks and several theoretic networks, and found that real networks are more heterogenous in the view of automorphism partition than what have been depicted under the measurement of degree-based entropy. We also found that structural heterogeneity measured by automorphism partition based-entropy is highly negatively correlated to the abundance of symmetry in real networks.

Generally, heterogeneity of networks is strongly correlated to the complexity of a network system, i.e., more het-

erogenous, more complex. Thus, we believe that precisely characterizing the heterogeneity of a network can definitely allow us to gain deeper insight into the complexity of systems represented by network.

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- [30] A *partition* of the set V is a set of disjoint non-empty subsets of V whose union is V . Elements of a partition are also called its *cells*. A *trivial cell* is the cell with cardinality one. If every cell of a partition is trivial, then the partition is a *discrete partition*; while if the partition only has one cell, the partition is a *unit partition*. For two partitions on set V , P and Q , if every cell of P is a subset of some cell of Q , we say that P is finer than Q , or Q is coarser than P .