An Entropic Edge Assortativity Measure

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Abstract. Assortativity or assortative mixing is the tendency of a network's vertices to connect to others with similar characteristics, and has been shown to play a vital role in the structural properties of complex networks. Most of the existing assortativity measures have been developed on the basis of vertex degree information. However, there is a significant amount of additional information residing in the edges in a network, such as the edge directionality and weights. Moreover, the von Neumann entropy has proved to be an efficient entropic complexity level characterization of the structural and functional properties of both undirected and directed networks. Hence, in this paper we aim to combine these two methods and propose a novel edge assortativity measure which quantifies the entropic preference of edges to form connections between similar vertices in undirected and directed graphs. We apply our novel assortativity characterization to both artificial random graphs and real-world networks. The experimental results demonstrate that our measure is effective in characterizing the structural complexity of networks and classifying networks that belong to different complexity classes.

Keywords: Assortative mixing · Von Neumann entropy · Entropic edge assortativity

1 Introduction

Over the past decade there has been a considerable interest in studying the properties of complex networks since they play a crucial role in revealing essential features of the structure, function and dynamics of many large-scale systems in biology, physics and the social sciences. To render such networks tractable, it is imperative to have to hand measures that efficiently reflect their structural, functional and dynamical diversity. An important example is the vertex degree assortativity, which expresses a bias in favor of connections between network vertices with similar degree [8]. Although the vertex degree provides a number of useful characterizations of network structure, significant information also resides in the edges of a network, including the direction of interaction between components and the information conveyed by a random walk on a network. In this paper we present an edge assortativity measure, making use of the von Neumann entropy, which is an effective structural complexity measure designed for complex networks [4][11].

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Assortativity is often formalized as a correlation between the degree distinction of two vertices in a graph. Recently, Foster et al. [3] have pointed out that the classification based on network assortativity is not always efficient for undirected networks. They further achieved that the fundamental feature of edge direction in a network also plays an important role. Thus they propose a set of four directed assortativity measures based on vertex in-degree and out-degree combinations. Recently, computing the importance of edges in a network has attracted considerable interest since many structural and functional features in networks have been shown to reside in the connections between vertices. For instance, the edge betweenness centrality, which is shown to be superior to graph planarization techniques, has been developed as an extension of betweenness centrality from vertices to edges [2].

The von Neumann entropy (or quantum entropy) associated with a density matrix, has proved to provide a highly effective complexity level characterization of a network. Han et al. [4] have taken this work further and have shown how to approximate the calculation of von Neumann entropy in terms of simple degree statistics rather than the normalized Laplacian eigenvalues. Recently, Ye et al. [11] have extended this entropy to the domain of directed graphs. In addition, the distribution of von Neumann entropy associated with edges in a graph, can be encoded as a multi-dimensional histogram, which not only captures the structure of a graph but also reflects its complexity [13] [12].

In this paper, we propose a novel edge assortativity measure based on the edge von Neumann entropy for both undirected and directed graphs. We use this measure to analyze how the entropy is distributed over edges. We show that the measure encodes a number of properties of the intrinsic structural properties of a graph, leading to the possibility of characterizing graphs of different structure.

The remainder of the paper is organized as follows. In Sec. II, we introduce briefly how the von Neumann entropy is defined and computationally simplified for both undirected and directed graphs. In Sec. III, we detail the development of the edge assortativity measure. In Sec. IV, we undertake experiments to demonstrate the usefulness of our method. Finally, in Sec. V we conclude our paper with a summary of our contribution and suggestions for future work.

2 Preliminaries

In this section, we give the definition of the von Neumann entropy for both undirected graph and directed graph, and show the entropy can be simplified in terms of edge entropy contributions.

2.1 Entropy Contribution for Undirected Edges

Suppose $G(V,E)$ is an undirected graph with vertex set V and edge set $E \subseteq V \times V$, then the adjacency matrix A is defined as follows

$$A_{uv} = \begin{cases} 1 & \text{if } (u, v) \in E \\ 0 & \text{otherwise.} \end{cases} \tag{1}$$

The degree of vertex u is $d_u = \sum_{v \in V} A_{uv}$.

According to [9], the normalized Laplacian matrix $\mathcal{L} = D^{-1/2}(D - A)D^{-1/2}$ (D is the degree matrix with the degree of the vertices of the undirected graph along the diagonal and zeros elsewhere) can be interpreted as the density matrix of an undirected graph. As a result, the undirected graph von Neumann entropy can be defined and calculated from the eigenvalues of the normalized Laplacian matrix. With this choice of density matrix, the von Neumann entropy of the undirected graph is the Shannon entropy associated with the normalized Laplacian eigenvalues, i.e., $H_{VN}^U = -\sum_{i=1}^{|V|}(\tilde{\lambda}_i/|V|)\ln(\tilde{\lambda}_i/|V|)$ where $\tilde{\lambda}_i$, $i = 1, \ldots, |V|$, are the eigenvalues of $\mathcal{L}$.

Commencing from this definition and making use of the quadratic approximation to the Shannon entropy, the von Neumann entropy can be approximated by a quadratic entropy [4] $H_Q^U = \sum_{i=1}^{|V|}\tilde{\lambda}_i/|V|(1 - \tilde{\lambda}_i/|V|)$, which can be expressed in terms of the trace of the normalized Laplacian (is equal to the sum of the normalized Laplacian eigenvalues) and the trace of the squared normalized Laplacian (is equal to the sum of the squares of the normalized Laplacian eigenvalues). Here, the accuracy of the above expression depends on the veracity of the quadratic approximation to the Shannon entropy $-x \ln x \approx x(1 - x)$. This approximation is known to hold well when either $x \to 0$ or $x \to 1$, which guarantees the accuracy of the quadratic entropy since $\tilde{\lambda}_i/|V| \to 0$ when the graph size is very large. Moreover, the trace of normalized Laplacian can be simply computed in terms of vertex degree in a graph, this leads to a more simplified form of the von Neumann entropy of an undirected graph:

$$H_{VN}^U = 1 - \frac{1}{|V|} - \frac{1}{|V|^2}\sum_{(u,v)\in E}\frac{1}{d_u d_v}. \tag{2}$$

This approximation clearly contains two measures of graph structure. The first term measures the effect of graph size and the second term of this formula simply calculates the sum of each edge contribution to the entropy of a graph. This leads to the possibility of defining a normalized local entropic measure for a single edge in the graph.

To this end, we normalize the von Neumann entropy with respect to the total number of edges in the graph in order to obtain the normalized edge entropy contribution, i.e.,

$$I_{uv}^U = \frac{1}{|V||E|d_u d_v}. \tag{3}$$

For an arbitrary graph, this normalized local entropic measure clearly avoids graph size bias and gives the von Neumann entropy contribution associated with each edge in the graph.

2.2 Entropy Contribution for Directed Edges

More recently, Ye et al. [11] have extended the calculation of von Neumann entropy from undirected graphs to directed graphs, using Chung's definition of the normalized Laplacian of a directed graph [1]. The resulting approximate entropy has the following form:

$$H_{VN}^{D} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\left(\frac{1}{d_u^{out}d_v^{out}} + \frac{d_u^{in}}{d_v^{in}d_u^{out^2}}\right) - \sum_{(u,v)\in E_u}\frac{1}{d_u^{out}d_v^{out}}\right\} \quad (4)$$

or equivalently,

$$H_{VN}^{D} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\left\{\sum_{(u,v)\in E}\frac{d_u^{in}}{d_v^{in}d_u^{out^2}} + \sum_{(u,v)\in E_b}\frac{1}{d_u^{out}d_v^{out}}\right\}, \quad (5)$$

where $E_u = \{(u,v)|(u,v) \in E \text{ and } (v,u) \notin E\}$ is the set of unidirectional edges while $E_b = \{(u,v)|(u,v) \in E \text{ and } (v,u) \in E\}$ is the set of bidirectional edges in the graph.

In particular, when $|E_u| \ll |E_b|$, i.e., few of the edges are unidirectional and the graph is weakly directed (WD), we ignore the summation over E_u in Eq.(4) in order to obtain the approximate von Neumann entropy for WD graphs:

$$H_{VN}^{WD} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\sum_{(u,v)\in E}\left\{\frac{\frac{d_u^{in}}{d_u^{out}} + \frac{d_v^{in}}{d_v^{out}}}{d_u^{out}d_v^{in}}\right\}. \quad (6)$$

The term $1 - \frac{1}{|V|}$ tends to unity as the graph size becomes large. In the summation, the numerator is given in terms of the sum of the ratios of in-degree and out-degree of the vertices. Since the directed edges cannot start at a sink (a vertex of zero out-degree), the ratios do not become infinite. Moreover, it is natural to realize that in our analysis an undirected graph is equivalent to a WD graph, since their von Neumann entropy expressions Eq.(2) and Eq.(6) are equivalent if we consider each undirected edge as a bidirectional one.

On the other hand, if the cardinality of E_b is very small ($|E_b| \ll |E_u|$), i.e., a graph is strongly directed (SD), this approximate entropy can be simplified one step further by ignoring the summation over E_b in Eq.(5):

$$H_{VN}^{SD} = 1 - \frac{1}{|V|} - \frac{1}{2|V|^2}\sum_{(u,v)\in E}\left\{\frac{d_u^{in}}{d_v^{in}d_u^{out^2}}\right\}. \quad (7)$$

This approximation clearly sums the entropy contribution from each directed edge, which is based on the in and out-degree statistics of the vertices connected by the edge. In other words, by using the same method in the previous subsection, we can compute a normalized local entropy measure for each directed edge in the SD graph. To do this, we remove the term $1 - \frac{1}{|V|}$ and normalize the remaining term with respect to the number of edges in the graph so that we obtain

$$I_{uv}^{D} = \frac{d_u^{in}}{|V||E|d_v^{in}d_u^{out2}} \quad (8)$$

as the von Neumann entropy contribution for edge $(u, v) \in E$.

3 Entropic Edge Assortativity Measure for Graphs

In this section, we propose a novel assortativity measure for both undirected and directed graphs based on the von Neumann entropy contributions associated with undirected and directed edges. This method provides useful underpinning at the use of entropy in determining graph structure. For instance, a high edge assortativity indicates that edges with large entropy associate preferentially and form some high entropy clusters in a graph. By contrast, a negative assortativity results from edges with high and low entropies that connect to each other.

The traditional assortativity is usually defined as the Pearson correlation coefficient (r) of the degrees of pairs of linked vertices [8]:

$$r = \frac{|E|^{-1}\sum_{(u,v)\in E} d_u d_v - [|E|^{-1}\sum_{(u,v)\in E}\frac{d_u+d_v}{2}]^2}{|E|^{-1}\sum_{(u,v)\in E}\frac{d_u^2+d_v^2}{2} - [|E|^{-1}\sum_{(u,v)\in E}\frac{d_u+d_v}{2}]^2} \in [-1, 1]. \quad (9)$$

When $r = 1$, the network is said to be perfectly assortative, when $r = 0$ the network is non-assortative, and when $r = -1$ the network is completely disassortative.

Furthermore, according to Foster et al. [3], in a directed graph, a set of four directed assortativity measures are defined as follows. Let $\alpha, \beta \in \{in, out\}$ be the directionality index for an edge at a vertex (i.e., whether it is incoming or outgoing). Then the directed assortativity measures are

$$r(\alpha, \beta) = \frac{|E|^{-1}\sum_{(u,v)\in E}[(d_u^\alpha - \bar{d_u^\alpha})(d_v^\beta - \bar{d_v^\beta})]}{\sigma^\alpha \sigma^\beta} \quad (10)$$

where $\bar{d_u^\alpha} = |E|^{-1}\sum_{(u,v)\in E} d_u^\alpha$ and $\sigma^\alpha = \sqrt{|E|^{-1}\sum_{(u,v)\in E}(d_u^\alpha - \bar{d_u^\alpha})^2}$; $\bar{d_v^\beta}$ and σ^β are similarly defined.

3.1 Entropic Edge Assortativity Measure for Undirected Graphs

Suppose $G(V, E)$ is an undirected graph, or equivalently, a weakly directed graph, then for an edge $(u, v) \in E$, we define the entropy contribution associated with the end vertex u of this edge S_{uv} as the summation of the entropies on the edges connected with u except the edge (u, v), i.e., $S_{uv} = \sum_{(t,u)\in E, t\neq v} I_{tu}^U$. The entropy contribution associated with another end vertex v is therefore $S_{vu} = \sum_{(v,w)\in E, w\neq u} I_{vw}^U$.

With these to hand, we define the edge assortativity as the Pearson correlation coefficient between all the entropy contributions associated with the two end vertices connected by the edge in the graph $G(V, E)$, with the result that

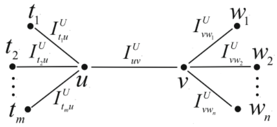


Fig. 1. The illustration of the calculation of quantities S_{uv} and S_{vu} associated with an undirected edge $(u, v) \in E$

$$R^U = \frac{\sum_{(u,v)\in E}(S_{uv} - \bar{S}_{uv})(S_{vu} - \bar{S}_{vu})}{\sigma_u^S \sigma_v^S} \tag{11}$$

where $\bar{S}_{uv} = |E|^{-1} \sum_{(u,v)\in E} S_{uv}$ and $\sigma_u^S = \sqrt{\sum_{(u,v)\in E}(S_{uv} - \bar{S}_{uv})^2}$; $\bar{S}_{vu}$ and σ_v^S are similarly defined. Clearly, this edge assortativity index provides a novel way to understand the entropic preference of edges to form connections between similar vertices in a graph.

3.2 Entropic Edge Assortativity Measure for Directed Graphs

We turn our attention to the domain of directed graphs. Here we mainly focus on the strongly directed graphs. Assume $G(V, E)$ is an SD graph, then for a directed edge starting from vertex u, ending at vertex v, we define the edge assortativity as the Pearson correlation coefficient between the edge entropy contribution H_{uv}^u associated with all the outgoing edges of vertex u (exclude edge (u, v)) and the contribution H_{uv}^v associated with all the incoming connections of vertex v (except edge (u, v)). The reason we use such definition is that this expression conforms to the structure of the approximate von Neumann entropy for SD graphs given in Eq.(7). Mathematically, we have $H_{uv}^u = \sum_{(u,s)\in E, s\neq v} I_{us}^D$ and $H_{uv}^v = \sum_{(p,v)\in E, p\neq u} I_{pv}^D$. Therefore the edge assortativity coefficient for SD graphs is given by

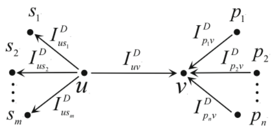


Fig. 2. The illustration of the calculation of quantities H_{uv}^u and H_{uv}^v associated with a directed edge $(u, v) \in E$

$$R^D = \frac{\sum_{(u,v)\in E}(H_{uv}^u - \bar{H}_{uv}^u)(H_{uv}^v - \bar{H}_{uv}^v)}{\sigma_u^H \sigma_v^H} \tag{12}$$

where $\bar{H}_{uv}^u = |E|^{-1} \sum_{(u,v)\in E} H_{uv}^u$ and $\sigma_u^H = \sqrt{\sum_{(u,v)\in E}(H_{uv}^u - \bar{H}_{uv}^u)^2}$; $\bar{H}_{uv}^v$ and σ_v^H are similarly defined. This measure is bounded between -1 and 1: a high coefficient of a graph indicates that most of the directed edges in the graph start from the vertex with outgoing edges that have high entropy contributions, and point to the vertex with incoming edges with high entropy contributions. Conversely, a negative coefficient results from most of the directed edges connect two vertices that have significantly different von Neumann edge entropy contributions.

4 Experiments and Discussion

We have proposed a novel edge assortativity characterization for quantifying the assortative mixing properties for both undirected and directed graphs based on the von Neumann entropy associated with edges. In this section, we explore whether this measure can reveal more useful features of the graph structure than the traditional degree assortativity measures. To this end, we confine our attention to two main tasks. We first apply the edge assortativity measure to some real-world complex networks to show that it can effectively reflect to what extent the vertices are connected preferentially in a network. We then demonstrate one advantage of this novel assortativity characterization, namely that it is more efficient in distinguishing between different classes of complex networks than the traditional measures.

4.1 Experiments and Discussion on Undirected Graphs

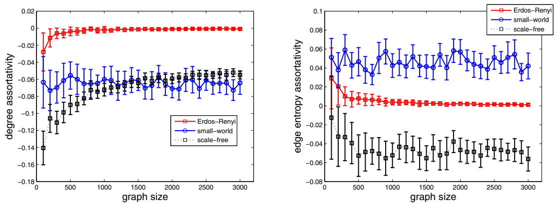
We commence by comparing the performance of traditional assortativity coefficients and our novel edge assortativity measure on real-world collaboration networks. These include the Arxiv Astro Physics, Condensed Matter, General Relativity, High Energy Physics and High Energy Physics Theory networks [7]. Table 1 gives the network size, edge number and value of both the degree and edge assortativity measures. From the table it is clear that all the coauthership networks have positive degree assortativity coefficients. This is a reasonable result since productive authors prefer to collaborate. However, the traditional assortativity coefficient has difficultly in distinguishing between CA-HepPh and CA-GrQc networks as their values are similar. The edge assortativity coefficient, on the other hand, is able to characterize these two networks. One of the reasons for this is that the edge assortativity measure can capture not only the degree properties of vertices, but also the underlying entropic structural complexity associated with the edges in a network.

Table 1. Degree assortativity coefficients and edge assortativity measures of real-world undirected complex networks

Datasets	HepTh	HepPh	GrQc	CondMat	AstroPh
Network size	9877	12008	5242	23133	18772
Edge number	51971	237010	28980	186936	396160
Degree assort.	0.2674	0.6322	0.6592	0.1339	0.2051
Edge entropy assort.	0.2012	0.6035	0.3910	0.3435	0.5458

Next we show that the edge assortativity measure is more efficient than the traditional assortativity coefficient in classifying graphs that belong to different random graph models. To do this we first randomly produce a large number of undirected graphs according to one of three models, namely a) the classical Erdős-Rényi model, b) the "small-world" model, and c) the "scale-free" model. The different graphs in the database are generated using a variety of model parameters, e.g. the graph size and the connection probability in the Erdős-Rényi model, the edge rewiring probability in the "small-world" model and the number of added connections at each time step in the "scale-free" model.

Figure 3 shows the mean value of both the degree assortativity coefficients (Eq.(9)) and edge assortativity measures (Eq.(11)) as a function of graph size (standard deviation as an error bar). In the left panel, all three classes of graphs tend to have zero assortative mixing when the graph size becomes very large, and it is difficult to separate the 'small-world" and "scale-free" graphs. Turning our attention to the right panel, the difference in mean edge assortativity coefficients for different models is much larger than the standard deviation of the coefficients for the different models, even when the graph size is large. This suggests that the variance in the edge assortativity measure due to different parameter settings is much smaller than that due to differences in structure. This indicates that different network models have different values of edge assortativity coefficients for a given size. This accords with our expectations since the entropy itself is sensitive to the different graph models.



(a) (b)

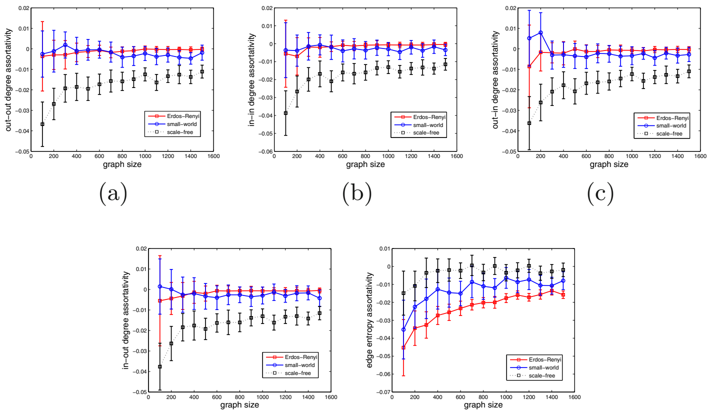
Fig. 3. Mean and standard deviation of vertex degree assortativity coefficients (Eq.(9)) and edge assortativity measures (Eq.(11)) for different models of undirected graphs. Red square solid line: Erdős-Rényi; blue circle solid line: "small-world"; black square dotted line: "scale-free".

4.2 Experiments and Discussion on Directed Graphs

For directed graphs, we first provide a comparison of our new directed edge assortativity measure, and the four assortativity coefficients that can be computed from the four combinations of in and out-degree on the two vertices of an edge. We commence with a study on some real-world networks, and these include the Wikipedia vote network, provided by Leskovec et al. [5], the Gnutella peer-to-peer networks from August 5 to 9, 2002, which are a sequence of snapshots of the Gnutella peer-to-peer file sharing network [10] and the Arxiv HEP-TH citation network [6]. Table 2 gives the network size, edge number and the values of in/in-degree, in/out-degree, out/in-degree, out/out-degree and edge assortativity measures. There are a number of observations concerning this data. In the Wikipedia vote network, a person who receives many votes is more likely to vote a person who also obtains a large number of votes, rather than voting for individuals who vote many times. In the file sharing networks, computers that receive a great number of documents preferentially share files with one-another. Computers that send many files are unlikely to share files with computers that receive many documents. For the citation network, important papers are those cited most heavily and this can be reflected accurately by the degree assortativity measures. Although when taken in combination the four types of directed

Table 2. Degree assortativity coefficients and edge assortativity measures of real-world directed complex networks

Datasets	Wiki-Vote	p2p-G05	p2p-G06	p2p-G08	p2p-G09	Arxiv HEP-TH
Network size	7115	8846	8717	6301	8114	27751
Edge number	103689	31839	31525	20777	26013	352807
In/in deg. assort.	0.0051	0.0312	0.0880	0.1079	0.1042	0.0405
In/out deg. assort.	0.0071	-0.0002	0.0322	0.0315	0.0190	0.0055
Out/in deg. assort.	-0.0832	-0.0034	-0.0032	-0.0285	-0.0327	0.0016
Out/out deg. assort.	-0.0161	-0.0017	0.0082	-0.0157	-0.0062	0.0951
Edge entropy assort.	0.0006	0.0053	-0.0092	-0.0038	-0.0055	0.1126



(a) (b) (c) (d) (e)

Fig. 4. Mean and standard deviation of vertex degree assortativity coefficients (Eq.(10)) and edge assortativity measures (Eq.(12)) for different models of directed graphs. Red square solid line: Erdős-Rényi; blue circle solid line: "small-world"; black square dotted line: "scale-free".

degree assortativity coefficients are useful in characterizing different networks, it is difficult to use a single measure alone to do this. However, when using the novel edge assortativity measure developed for directed graphs, networks with different structures are efficiently characterized.

In Fig. 4 we plot the values of the edge assortativity coefficient, and compare them to the assortativity coefficients obtained with the four different combinations of vertex in and out-degree on an edge (see Eq.(10)). Here we use randomly generated data for three different directed graph models. The figure shows the assortativity measures versus graph size, and shows the mean value and standard deviation. The most important feature in the figure is that although the "scale-free" networks are easily separated, the Erdős-Rényi and "small-world" networks are overlapped significantly, for each of the four degree assortativity coefficients. However, Fig. 4(e) suggests that as the graph size increases, for all three models the mean values of the edge assortativity measures grow slowly and approach zero, with clear separations between them. The result obtained here demonstrates that the edge assortativity measure provides a powerful tool for capturing both the degree properties and the entropic information on edges in a directed network.

5 Conclusions

To conclude, this paper is motivated by the aim of proposing novel measures that quantify the assortative mixing properties for both undirected and directed networks. We commence from the recently developed simplified approximations to the von Neumann entropy for both undirected and directed graphs, which are dependent on the graph size and degree statistics of vertices that are connected. From these approximations we then derive a local measure for quantifying the von Neumann entropy contribution for each edge in the undirected and directed graph respectively. This leads to the possibility of designing a correlation coefficient that measures the average assortative properties of how the entropy contributions that reside in edges are connected in a network, which we name the edge assortativity measure. The resulting expressions for such measures of both undirected and directed graphs are simply related to some graph invariants, including the graph size, number of edges and the vertex degree.

The work reported in this paper can be extended in a number of ways. First, it would be interesting to explore how the distribution of the edge entropy contributions in a network can contribute to the development of novel information theoretic divergence, distance measures and relative entropies. Another interesting line of investigation would be to investigate whether this measure can be applied further to weighted graphs and hypergraphs.

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