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The clustergram: A graph for visualizing hierarchical and nonhierarchical cluster analyses

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Abstract. In hierarchical cluster analysis, dendrograms are used to visualize how clusters are formed. I propose an alternative graph called a “clustergram” to examine how cluster members are assigned to clusters as the number of clusters increases. This graph is useful in exploratory analysis for nonhierarchical clustering algorithms such as k -means and for hierarchical cluster algorithms when the number of observations is large enough to make dendrograms impractical. I present the Stata code and give two examples.

Keywords: st0028, dendrogram, tree, clustering, nonhierarchical, large data, asbestos

1 Introduction

The *Academic Press Dictionary of Science and Technology* defines a dendrogram as follows:

dendrogram *Biology.* a branching diagram used to show relationships between members of a group; a family tree with the oldest common ancestor at the base, and branches for various divisions of lineage.

In cluster analysis, a dendrogram (see [R] **cluster dendrogram** and, for example, Everitt and Dunn 1991 and Johnson and Wichern 1988) is a tree graph that can be used to examine how clusters are formed in hierarchical cluster analysis (see [R] **cluster singlelinkage**, [R] **cluster completelinkage**, [R] **cluster averagelinkage**). Figure 1 gives an example of a dendrogram with 75 observations. Each leaf represents an individual observation. The leaves are spaced evenly along the horizontal axis. The vertical axis indicates a distance or dissimilarity measure. The height of a node represents the distance of the two clusters that the node joins. The graph is used to visualize how clusters are formed. For example, if the maximal distance on the y -axis is set to 40, then three clusters are formed because $y = 40$ intersects the tree three times.

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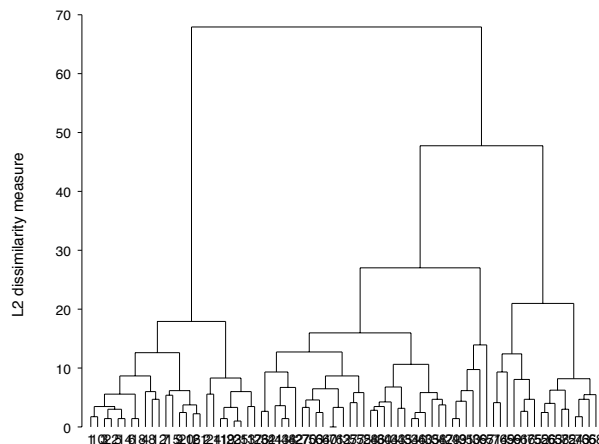


Figure 1: A dendrogram for 75 observations

Dendrograms have two key limitations. First, because each observation must be displayed as a leaf, they can only be used for a small number of observations. Stata 7 allows up to 100 observations. As Figure 1 shows, even with 75 observations, it is difficult to distinguish individual leaves. Second, the vertical axis represents the level of the criterion at which any two clusters can be joined. Successive joining of clusters implies a hierarchical structure, meaning that dendrograms are only suitable for hierarchical cluster analyses.

For large numbers of observations, hierarchical cluster algorithms can be too time-consuming. The computational complexity of the three popular linkage methods is of order $O(n^2)$, whereas the most popular nonhierarchical cluster algorithm, k -means ([R] **cluster kmeans**; MacQueen 1967), is only of the order $O(kn)$. Here, k is the number of clusters, and n is the number of observations (Hand, Mannila, and Smyth 2001). Therefore, k -means, a nonhierarchical method, is emerging as a popular choice in the data mining community.

I propose a graph that examines how cluster members are assigned to clusters as the number of clusters changes. In this way, it is similar to the dendrogram. Unlike the dendrogram, this graph can also be used for nonhierarchical clustering algorithms. I call this graph a clustergram.

The outline of the remainder of this paper is as follows: Section 2 describes the syntax and options of the new Stata command **clustergram**. Section 3 explains how the clustergram is computed by means of an example related to asbestos lawsuits. The example also illustrates the use of the **clustergram** command. Section 4 contains a second example: Fisher's famous *Iris* data. Section 5 concludes with some discussion.

2 Syntax

```
clustergram varlist [if exp] [in range] , cluster(clustervarlist) [fraction(#)  
fill graph_options]
```

Here *varlist* contains variables that are being clustered and must be supplied. I illustrate this in an example below.

3 Options

`cluster(clustervarlist)` specifies the variables containing cluster assignments, as previously produced by `cluster`. More precisely, they usually successively specify assignments to 1, 2, ... clusters. Typically, they will be named something like `cluster1-cluster max` , where *max* is the maximum number of clusters identified. It is possible to specify assignments other than to 1, 2, ... clusters (e.g., omitting the first few clusters or in reverse order). A warning will be displayed in this case. This option is required.

`fraction(#)` specifies a fudge factor controlling the width of line segments and is typically modified to reduce visual clutter. The relative width of any two line segments is not affected. The value should be between 0 and 1. The default is 0.2.

`fill` specifies that individual graph segments are to be filled (solid). By default, only the outline of each segment is drawn.

graph_options are options of `graph`, `twoway` other than `symbol()` and `connect()`. The defaults include `ylabels` showing three (rounded) levels and `gap(5)`.

4 Description and the asbestos data example

A huge number of lawsuits concerning asbestos-related personal injuries have been filed in the United States. One interesting question is “Can companies be clustered into groups on the basis of how many lawsuits were filed against them?” The data consist of the number of asbestos suits filed against 178 companies in the United States from 1970 through 2000. Figure 2 shows a plot of the log base 10 of the number of asbestos suits over time for each of the 178 companies. Few asbestos lawsuits were filed in the early years. By 1990, some companies were subject to 10,000 asbestos-related lawsuits in a single year. I separate the number of asbestos suits by year to create 31 variables for the cluster algorithm. Each variable consists of the log base 10 of the number of suits that were filed against a company in a year.

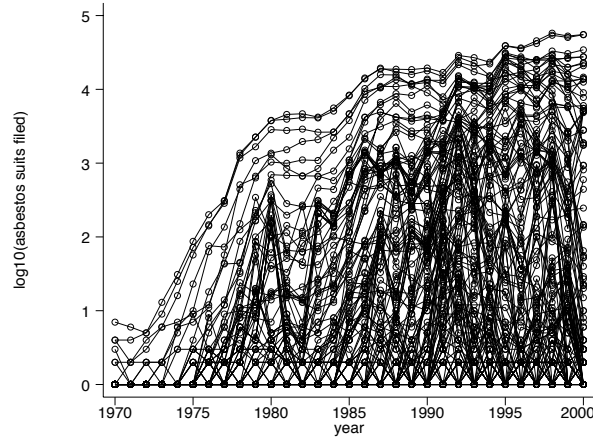


Figure 2: Plot of the log base 10 number of asbestos suits over time for each of the 178 companies

A principal components analysis of the covariance matrix of these 31 variables shows that the first principal component captures 82% and that the second principal component captures 7% of the variation. The first principal component consists of a weighted average of all variables, with larger weights attributed to years with more lawsuits (approximately 1978–2000). Clearly, it is an overall measure of the number of lawsuits. The second principal component consists of a contrast between variables corresponding to 1978–1992 and those corresponding to 1993–2000. This component captures whether the number of lawsuits continued to increase, stagnate, or decrease during these years. Figure 3 shows a scatter plot of the first two principal components. The cluster at the bottom consists of companies with none or few lawsuits.

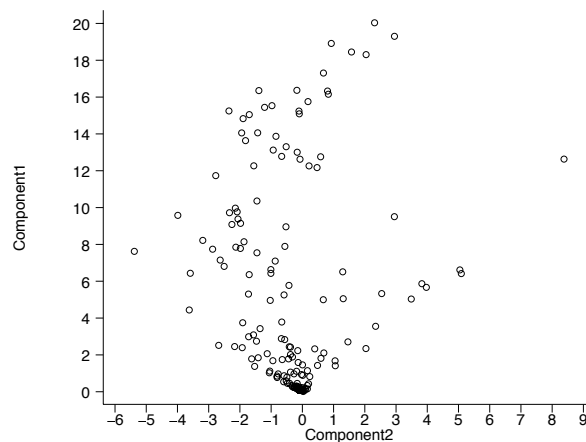


Figure 3: Scatter plot of the first two principal components

In preparation for constructing the clustergram, the chosen cluster algorithm must be run multiple times, each time specifying a different number of clusters (e.g., 1 through 20). For example, 20 cluster variables can be created named `cluster1` through `cluster20`, using the k -means clustering algorithm in Stata as follows:

```
. forvalues i = 1/20 {
.     cluster kmeans log1970-log2000, k('i') L1 name("cluster'i'")
. }
```

These variables are needed as inputs for the clustergram. The clustergram is constructed as follows: For each cluster within each cluster analysis, compute the mean over all cluster variables and over all observations in that cluster. For example, for $x = 2$ clusters, compute two cluster means. For each cluster, plot the cluster mean versus the number of clusters. Connect cluster means of consecutive cluster analyses with parallelograms. The width of each parallelogram indicates how many observations from a cluster were assigned to a cluster in the following cluster analysis.

Figure 4 illustrates this. Initially, all observations form a single cluster. This cluster is split into two clusters. The lower parallelogram is much thicker than the upper one, indicating that many more observations fall into the lower cluster. These two clusters are then split into three clusters. A new cluster is formed in the middle, which draws some observations that were previously classified in the lower cluster, and some that were previously classified in the higher cluster. Because the new cluster is formed from observations of more than one previous cluster (i.e., has more than one parent), this is a nonhierarchical split. On the vertical axis, the log base 10 of the average number of lawsuits filed against a company is shown. Therefore, “higher” or “lower” clusters refer to clusters with companies that on average have a larger or smaller number of lawsuits.

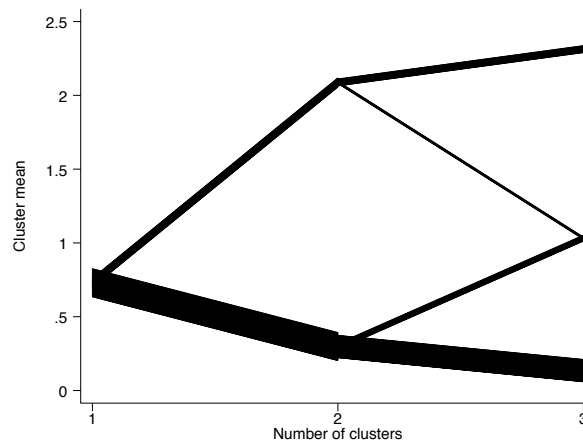


Figure 4: A clustergram for 1 to 3 clusters. The cluster assignments stem from the k -means algorithm.

To avoid visual clutter, the width of all parallelograms or graph segments can be controlled through a fudge factor. This factor by default is 0.2 and can optionally be set by the user. The amount should be chosen large enough that clusters of various sizes can be distinguished, and small enough that there is not too much visual clutter.

Using the syntax introduced in Section 2, the clustergram with up to 20 different clusters can be obtained as follows:

```
. clustergram log1970-log2000, cluster(cluster1-cluster20) fraction(0.1)
> xlab(1 2 to 20) ylab(0 0.5 to 3.5) fill
```

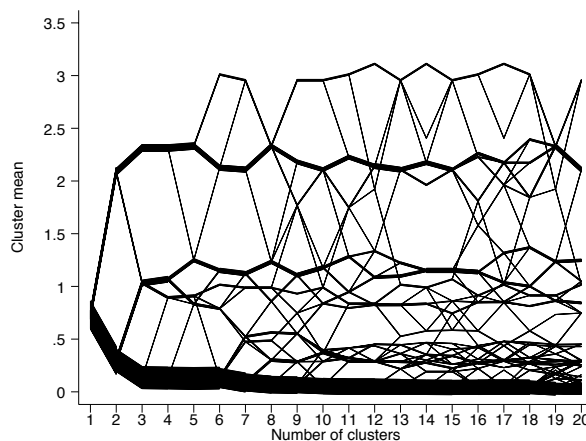


Figure 5: Clustergram with up to 20 clusters. The k -means cluster algorithm was used.

Figure 5 displays the resulting clustergram for up to 20 clusters. We see that the companies initially split into two clusters of unequal size. The cluster with the lowest mean remains the largest cluster by far for all cluster sizes. One can also identify hierarchical splits. A split is a hierarchical split when a cluster has only one parent or predecessor. The split from 3 to 4 clusters is almost hierarchical (it is not strictly hierarchical because a single company joins from the bottom cluster). Also, there are a number of individual companies that appear to be hard to classify because they switch clusters.

At 8 and 19 clusters, the two clusters at the top merge and then split again. This highlights a weakness of the k -means algorithm. For some starting values, the algorithm may not find the best solution. The clustergram in this case is able to identify the instability for this dataset.

Figure 6 shows a clustergram for a hierarchical, average linkage cluster analysis. These were obtained using the following Stata commands:

```
. cluster averagelinkage log1970-log2000, L1 name("clusX")
. forvalues i = 1/20 {
.     cluster gen cluster'i' = group('i')
. }
```

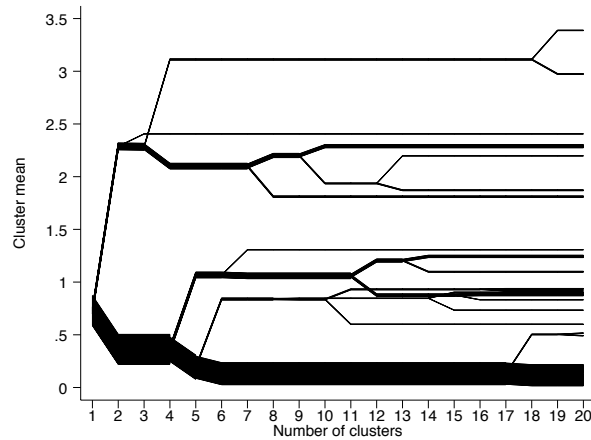


Figure 6: A clustergram for an average linkage (hierarchical) cluster analysis.

Because of the hierarchical nature of the algorithm, once a cluster is split off, it cannot later join with other clusters. Qualitatively, Figure 5 and Figure 6 convey the same picture. Again, the bottom cluster has by far the most members, and the other two or three major streams of clusters appear at roughly the same time with a very similar mean.

In Figure 7, we see a clustergram for a hierarchical, single linkage cluster analysis. Most clusters are formed by splitting a single company off the largest cluster. When the 11th cluster is formed, the largest cluster shifts visibly downward. Unlike most of the previous new clusters, the 11th cluster has more than one member, and its cluster mean of about 2.5 is relatively large. The reassignment of these companies to the 11th cluster causes the mean of the largest cluster to drop visibly. If our goal is to identify several nontrivial clusters, this cluster algorithm does not suit this purpose. Figure 7 conveys this information instantly.

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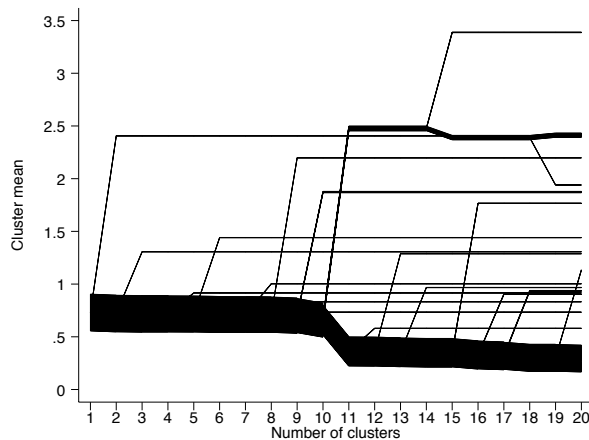


Figure 7: A clustergram for a single linkage (hierarchical) cluster analysis.

Of course, the ultimate decision on the number of clusters is always somewhat arbitrary and should be based on subject-matter expertise and the criterion that measures within-cluster homogeneity, as well as on insight gained from the clustergrams. It is re-assuring that k -means and the average linkage algorithm lead to qualitatively similar results.

5 Iris data example

Fisher's *Iris* data (Fisher 1938) consists of four variables: length and width of sepal and petal of *Iris*. It is known that there are three different species of *Iris*, namely *Iris setosa*, *Iris versicolor*, and *Iris virginica*.

It is of interest whether one can distinguish these species based on these four variables. Figure 8 shows a scatter plot of petal length and width. This scatter plot best shows how the three species are separated. One species is relatively easy to distinguish from the other two; distinguishing between the other two is harder. Because the data consist of 150 observations, a full dendrogram cannot be drawn in Stata.

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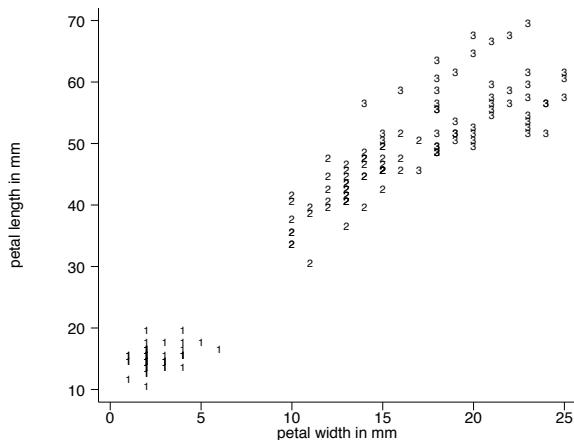


Figure 8: Scatter plot of petal width and petal length of the *Iris* data. Different plotting symbols indicate different species: (1) *Iris setosa*, (2) *Iris versicolor*, and (3) *Iris virginica*.

Figure 9 shows clustergrams for the *k*-means algorithm and the three linkage algorithms for cluster analyses on the standardized dataset. The initial splits for the *k*-means, average and single linkage algorithms look identical, and this turns out to be true. At the initial split, species 1 (numbers as labeled in Figure 8) is separated from species 2 and 3, which form a joint cluster. As we have seen in Figure 8, species 1 has lower *x* values, and therefore, the species 1 cluster corresponds to the lower branch in Figure 9. As we have seen in Figure 7, the single linkage cluster algorithm has a tendency to split off single observations. The fact that here the single linkage algorithm forms two clusters of substantial size suggests that the clusters are well separated. This is true, as we have seen in Figure 8. Because of its distance criterion (the maximum distance between any two members of two clusters), the complete linkage cluster algorithm tends to avoid elongated clusters in favor of more compact clusters. Here, the complete cluster algorithm splits the elongated data cloud roughly in half.

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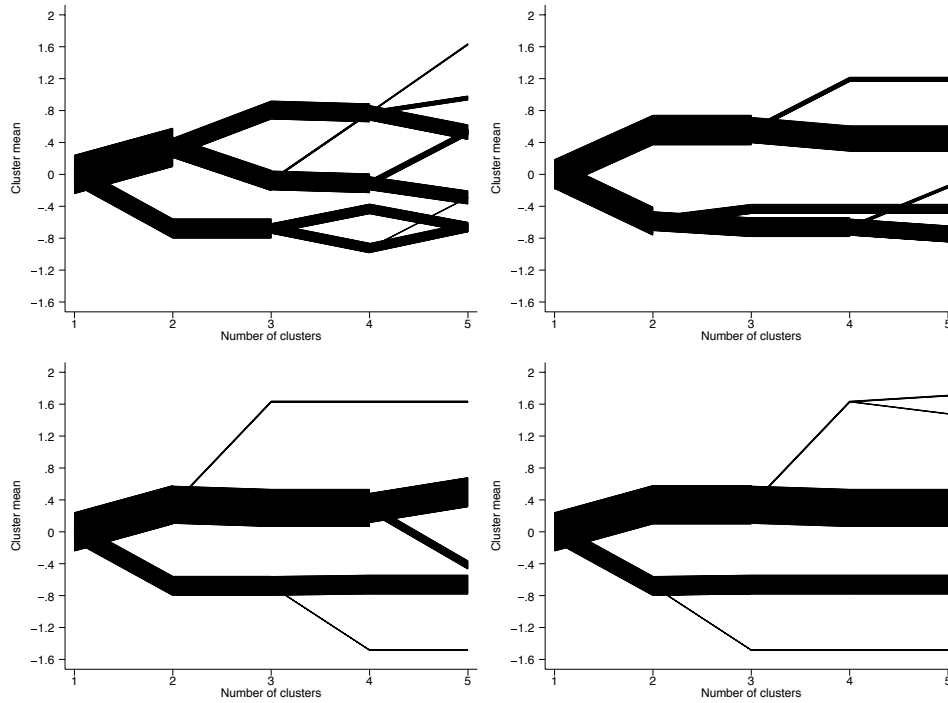


Figure 9: Clustergram for four cluster analyses on the *Iris* data: k -means (upper left), complete linkage (upper right), average linkage (lower left), and single linkage (lower right).

When three clusters are formed, the k -means algorithm breaks the cluster consisting of species 2 and 3 into separate clusters. By contrast, Figure 9 shows that the average and single linkage cluster algorithm split off a small number of observations. The complete linkage algorithm splits the lower cluster, attempting to separate species 1 from other observations.

Table 1 displays the confusion matrix (the matrix of misclassifications) for each of the four algorithms based on three clusters. k -means has the best classification rate, classifying 83% of the observations correctly. However, the success of the k -means algorithm depends on one of the initial cluster seeds falling into the cloud of species 1 observations. Surprisingly, the complete linkage algorithm has the second best classification rate. Given its poor first split, the second split is nearly perfect. The single linkage algorithm is confused by the proximity of species 2 and 3. The algorithm incorrectly chooses to split a single observation off the pure cluster consisting of species 1.

Table 1: Confusion matrix for several cluster algorithms on Fisher's *Iris* data

		Cluster 1	Cluster 2	Cluster 3
k-means				
83% correctly classified	Species 1	50	0	0
	Species 2	0	39	11
	Species 3	0	14	36
Complete Linkage				
79% correctly classified	Species 1	49	1	0
	Species 2	0	21	29
	Species 3	0	2	48
Average Linkage				
69% correctly classified	Species 1	50	0	0
	Species 2	0	50	0
	Species 3	0	47	3
Single Linkage				
66% correctly classified	Species 1	49	0	1
	Species 2	0	50	0
	Species 3	0	50	0

6 Discussion

The clustergram is able to highlight quickly a number of things that may be helpful in deciding which cluster algorithm to use and/or how many clusters may be appropriate: approximate size of clusters, including singleton clusters (clusters with only one member); hierarchical versus nonhierarchical cluster splits; hard to classify observations; and the stability of the cluster means as the number of clusters increase.

For cluster analysis, it is generally recommended that the cluster variables be on the same scale. Because means are computed, this is also true for the clustergram. In the asbestos claims example, all variables measured the same quantity: the number of lawsuits in a given year. For most other applications—including Fisher's *Iris* data—it is best to standardize the variables.

The dendrogram is a hierarchical, binary tree in which each branch represents a cluster. (Strictly, it need not be binary; in the rare case of ties, a node can have more than two children.) Ultimately, at the leaves of the tree, each observation becomes its own cluster. The clustergram is a nonhierarchical tree. The number of branches varies and can be as large as the number of clusters. For example, observations in one of the clusters at $x = 10$ can branch out into any of the 11 clusters at $x = 11$. We have only looked at up to 20 clusters. If one were to continue to increase the number of clusters up to the point where the number of clusters equals the number of observations, then at the leaves, each cluster would consist of only one observation.

The clustergram differs from the dendrogram as follows: First, the layout on the dendrogram's horizontal axis is naturally determined by the tree (except for some freedom in whether to label a branch left or right). The layout of the nonhierarchical tree is not obvious. We chose to use the mean to determine the coordinate. Other functions are possible. Second, in the dendrogram, "distance" is used as the second axis. "Distance" naturally determines the number of clusters. In the clustergram, we use the number of clusters instead. Third, in a clustergram, the (nonhierarchical) tree is not usually extended until each leaf contains only one observation. Fourth, in a clustergram, the width of the parallelogram indicates cluster size. This is not necessary for the dendrogram. Because all leaves are plotted uniformly across the horizontal axis, the width of the cluster already gives a visual cue as to its size.

The clustergram can be used for hierarchical clusters. If the dataset is small enough to display a full dendrogram, a dendrogram is preferable because "distance" conveys more information than "number of clusters".

7 Acknowledgement

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8 References

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