Clustering Big Data

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Abstract: The need to support advanced analytics on Big Data is driving data scientist' interest toward massively parallel distributed systems and software platforms, such as Map-Reduce and Spark, that make possible their scalable utilization. However, when complex data mining algorithms are required, their fully scalable deployment on such platforms faces a number of technical challenges that grow with the complexity of the algorithms involved. Thus algorithms, that were originally designed for a sequential nature, must often be redesigned in order to effectively use the distributed computational resources. In this paper, we explore these problems, and then propose a solution which has proven to be very effective on the complex hierarchical clustering algorithm CLUBS+. By using four stages of successive refinements, CLUBS+ delivers high-quality clusters of data grouped around their centroids, working in a totally unsupervised fashion. Experimental results confirm the accuracy and scalability of CLUBS+ on Map-Reduce platforms.

1 INTRODUCTION

The current era of *Big Data* (Nature, 2008) has forced both researchers and industries to rethink the computational solutions for analyzing massive data. In fact, a great deal of attention has been devoted to the design of new algorithms for analyzing information available from Twitter, Google, Facebook, and Wikipedia, just to cite a few of the main big data producers. Although this massive volume of data can be quite useful for people and companies, it makes analytical and retrieval operations really time consuming due to their high computational cost. A possible solution relies upon the opportunity to cluster big data in a compact but still informative version of the entire data set. Obviously, such clustering techniques should produce clusters (or summaries) having high accuracy. Clustering algorithms could be beneficial in several application scenarios such as cybersecurity, user profiling and recommendation systems, to cite a few. Although all textbooks describe clustering as the quintessential "unsupervised learning task" all the major algorithms proposed so far require significant guidance from the user, such as the number of clusters to be derived for *k*-means++ and the termination condition for hierarchical clustering. In (Mazzeo et al., 2017) the authors proposed CLUBS$^+$, a clustering algorithm that manages to be very effective without any user guidance by (i) operating in multiple stages whereby the techniques used at one stage compensate for the shortcomings of the previous stages, and by (ii) applying carefully selected and well-tuned criteria to assure the quality of the results produced at each stage. In particular, the benefit of (i), is illustrated by the fact that while over-splitting represents a very difficult issue for most divisive algorithms, it is much less of concern here, because a certain degree of over-splitting can be tolerated since it will be undone in the successive stages that include an agglomerative step.

In this paper we present a parallel version of CLUBS$^+$, which we call CLUBS-P. Like CLUBS$^+$, CLUBS-P, scales linearly w.r.t. the size of the data set. Furthermore, experiments show that the speed-up increases almost linearly as more machines for running the algorithm are available. These two features make CLUBS-P a very effective algorithm for clustering large amount of data. Finally, a nice feature of CLUBS-P is that once the data set to be clustered has been distributed across the available machines, there is no need to move data, as CLUBS-P requires the machines to exchange only summary information.

We provided a new implementation of our parallel

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clustering algorithm, based on the widely used Big Data framework Apache Spark (Zaharia et al., 2010).

The implementation of a distributed algorithm calls for suitable solution to some crucial problem in a distributed programming environment such as: load balancing and fault tolerance. A very popular solution proposed in recent years for implementing parallel algorithms tailored for Big Data is Apache Spark[1]. Indeed, it offers very useful functions which relieves the programmers from the explicit management of process assignment and memory management. In this respect, we implemented our CLUBS-P algorithm based on Spark. This paper is organized as follows. In Section 2 we provide an overview of CLUBS$^+$, while in Section 3 we first discuss the crucial points of CLUBS$^+$ with a view to its parallelization, that lead to devising CLUBS-P, for which we present a new implementation based on Apache Spark (Section 4). In Section 5 we present the experimental results and, finally, in Section 6 we draw our conclusions.

2 AN OVERVIEW OF CLUBS$^+$

In (Mazzeo et al., 2017) the authors introduced CLUBS$^+$. It is a parameter-free around-centroid clustering algorithm based on a fast hierarchical approach, that combines the benefits of the divisive and agglomerative approaches. The first operation performed by CLUBS$^+$ is the definition of a binary space partition of the domain of the dataset D, which yields set of coarse clusters that are then refined. The next operation is an agglomerative procedure performed over the previously refined clusters, which is followed by a final refinement phase. In the refinement phases, outliers are identified and the remaining points are assigned to the nearest cluster. In our running example of Fig. 1, we show how the successive steps of CLUBS$^+$ applied to the two-dimensional data distribution of Fig. 1(a), produce the results shown in Fig. 1(b–e). In order to make this paper-self contained, in the following we provide some details about the four steps of CLUBS$^+$ allowing a full comprehension of the parallel algorithm implemented in this paper, while a more exhaustive description of the algorithm phases can be found in (Mazzeo et al., 2017).

The *divisive step* of CLUBS$^+$ performs a top-down binary partitioning of the data set to isolate hyper-rectangular blocks whose points are as much as possible close to each other: this is equivalent to minimizing the *within clusters sum of squares* (*WCSS*) of the blocks, an objective also pursued by k-means and many other algorithms.

[1]http://spark.apache.org/

Since finding the partitioning which minimizes a measure such as the *WCSS* is NP-hard even for two-dimensional points (Muthukrishnan et al., 1999), CLUBS$^+$ uses a greedy approach where the splitting hyperplanes are orthogonal to the dimension axes, and the blocks are recursively split into pairs of clusters that optimize specific clustering criteria that will be discussed later. Given a input dataset, the algorithm begins with a single cluster S corresponding to the whole data set. S is entered into a priority queue, Q. Q contains blocks of the partition that is iteratively build over the dataset. While Q is not empty, a block B is removed and split into a pair of blocks. If the split is effective, the pairs of blocks replace B in Q, otherwise B becomes a 'final' block for this phase.

In order to efficiently find the best split for a block, the marginal distributions of the block must be computed. In particular, for each dimension i of a d-dimensional block B we must compute the functions $C^i_B : \mathbb{R} \rightarrow \mathbb{N}$ and $LS^i_B : \mathbb{R} \rightarrow \mathbb{R}^d$, defined as follows

$$C^i_B(x) = |p \in B \wedge p[i] = x| \quad (1)$$

$$LS^i_B(x) = \sum_{p \in B \wedge p[i]=x} p \quad (2)$$

where $p[i]$ is the i-th coordinate of the point p. These functions can be represented as maps, or, assuming that the coordinates of the points are integers, as arrays. In (Mazzeo et al., 2017) the authors showed that the split that minimizes the *WCSS* can be found through a linear scan of these maps/arrays. The authors conducted an extensive evaluation of the effectiveness of criteria proposed in the literature for estimating the quality and naturalness of a cluster set (Arbelaitz et al., 2013), and they concluded that the Calinski-Harabasz index, *CH-index* for short, is the most suitable to their needs (Calinski and Harabasz, 1974). Briefly, after each step, we compute the new *CH-index*, and if it is increased by the split, then we consider the split effective and continue the divisive phase. Otherwise, we check a "local" criterion, based on the presence of a 'valley' in the marginal distribution. In fact, even though a split could not decrease the overall *CH-index*, a very large local discontinuity could justify the split of a block anyway.

When the divisive phase is completed, the overall space is partitioned into (a) blocks containing clusters, and (b) blocks that only contain noise points. In this *intermediate refinement* phase CLUBS$^+$ seeks to achieve the objectives of (I) separating the blocks that contain clusters from those that do not, and (II) generating well-rounded clusters for the blocks in the previous group.

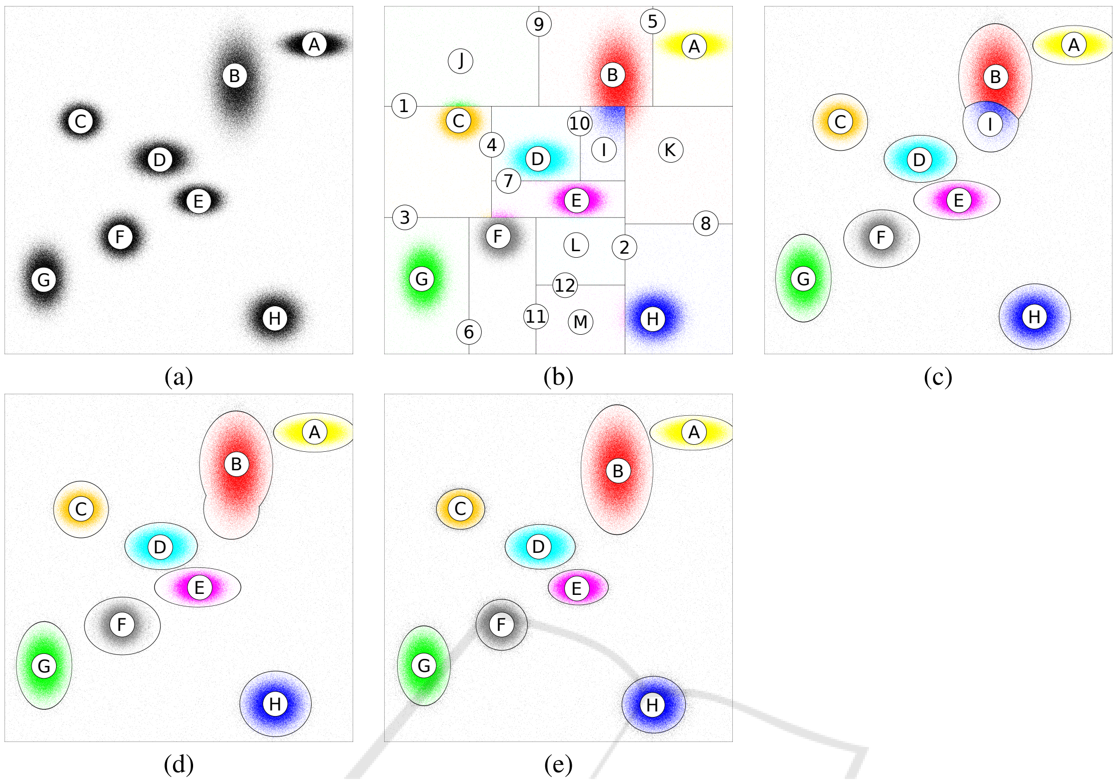


Figure 1: A two-dimensional data set with 8 clusters (a), its partitioning after the divisive step (b), the intermediate refinement (c), the agglomerative step (d), and the final refinement (e).

Task (I) is performed by using the observation that (a) the density of blocks containing only noise is low, and (b) the density of such blocks is rather uniform because of the random nature of noise.

For instance, these tests applied to our running example in Fig. 1(b) have classified blocks “J”, “K”, “L” and “M” as outlier-blocks.

Once, the cluster-blocks have been found, we can now proceed with task (II).

This step produces well-rounded clusters that restore the natural clusters that might have been shaved-off by rigid partitioning scheme leveraged in the divisive step. For instance, the block of data in Fig. 1(b), which contains the points of the cluster “E” in Fig. 1(a), contains also some points of the original cluster “F” which is now reassembled about its centroid.

In the *agglomerative step*, the clusters produced by the previous step are merged whenever this improves the overall clustering quality. The process of merging is symmetric to that of splitting: at each step we find the pair of clusters whose merge produces the least increase of *WCSS* and, if *CH-index* resulting from their merge increases, the merge is actually performed by replacing the two clusters by their union. If we determine that merging these two clusters will decrease the *CH-index*, the merge is not performed and the whole agglomerative phase ends, since no merging of other cluster pair can improve *CH-index*.

Fig. 1(d) shows that the the cluster “B” is obtained as the merge of the clusters “B” and “I” of Fig. 1(c).

The agglomerative step is a very fast step, as does not require to access data, since it is based only on previously computed summary information.

The *agglomerative step* often produces clusters of slightly irregular shapes due to the approximate and greedy criteria used in the previous steps. For instance, Fig. 1(d) shows that cluster “B” has been obtained by merging clusters “B” and “I” of Fig. 1(c). The evident asymmetry is due to the fact that the block “K” of Fig. 1(b) has been considered an outlier-block during the intermediate refinement, and the points at its upper-left corner have been asymmetrically adsorbed (due to their different position and radius) by blocks “B” and “I”.

The final refinement step improves the quality of clusters and also identifies the final outlier points.

The algorithm used to perform final refinement is basically the same as the one used for task (II) of the intermediate refinement (see (Mazzeo et al., 2017) for further details).

3 CLUBS-P: THE PARALLELIZATION OF CLUBS$^+$

We now analyze the steps of CLUBS$^+$ with the aim of pointing out the issues to be tackled in order to parallelize its execution.

We assume that n workers (i.e., different machines) with equivalent hardware features are available. The workers are coordinated by a master machine. The dataset is distributed over the worker nodes that store locally a portion of the dataset, which can be, for instance stored, in a distributed file system, or even previously split over the local file systems of the machines.

It is quite intuitive that the critical operations that can benefit from the availability of multiple workers are those requiring to access the original data: 1) computation of the marginal distributions during the divisive phase; 2) computation of the local density of outlier blocks candidates during the intermediate refinement; 3) assignment of points to the closest centroid during the refinement phases;

The parallelization of the operations above is discussed in the following. The other operations, which involves computations on summary information, instead, can be handled by the master, using the same approach as in the original version of CLUBS$^+$.

3.1 Parallel Computation of the Marginal Distributions

As remarked in previous section, the computation of the marginal distributions, more specifically of the vectors C and LS, is the only operation that requires to access the data during the divisive step. This operation can be efficiently performed in parallel thanks to the associativity and commutativity of the sum and count operations, which are the only mathematical operations involved in the computation. Therefore, given a block partition of the data B, $\{B_1, \ldots B_k\}$, those vectors can be independently computed on each B_i (thus in parallel) and the vector for the whole block B can be obtained by simply summing the vectors obtained on all the B_i. According to the Map-Reduce paradigm, each block B_i is mapped to a set of pairs of vectors, representing its C and LS for each dimension, and these vectors are subsequently reduced by summing vectors of the same dimension.

3.2 Parallel Computation of the Local Density of the Blocks

The local density of blocks has to be computed in order to evaluate the criterion used for Task II of the intermediate refinement. After the master has the list of the blocks resulting from the divisive phase, it also has their ranges and their global density. In order to check if the local density around the centroid of each block is significantly higher than the global density, it computes the boundaries of a small range around the centroid (i.e., a range of size $1/10$ of the whole block range), and then coordinates the parallel computation of the count of the points falling in each of these 'restricted' ranges. Even in this case, the only mathematical operation involved in the computation is sum, thus the operation is perfectly parallelizable. In fact, for each portion of data of a block, it is possible to independently compute the count of points laying in the restricted range, and then the overall count is simply given by the sum of the partial counts. This count allows the master to compute the local density, and thus apply the criterion described above.

3.3 Parallel Assignment of the Points to the Clusters

The assigment of the points to the clusters, or their classification as outliers, is an operation performed in both the refinement steps. Each worker can perform this operation independently on the others. The master, which has the summary information about the clusters, needs to send to every worker the information needed to compute the distance between points and clusters. After the computation, the same information must be updated by the master, since the cluster assignment of some points is likely to change. To this end, each node can compute the summary information for its data, and then, again, the master can simply obtain the global values of the new centroids, number of points per cluster, and cluster radius, after summing up all the values obtained from the workers.

We presented the general ideas on which our 'abstract' algorithm CLUBS-P is based for the parallelization of CLUBS. In the following, we propose a new implementation of this algorithm, using the Apache Spark. The implementation is available as open source software [2].

4 CLUBS-P MEETS SPARK: CLUBS*

The implementation of a distributed algorithm requires a lot of effort for solving specific issues related to the problem, but also general issues for distributed computing, such as load balancing and fault tolerance. Nowadays, a very popular framework for im-

[2]https://github.com/gmmazzeo/clubspark

plementing parallel algorithms tailored for Big Data is Apache Spark[3]. As a matter of fact, it offers very useful functions which relieves the programmers from the burden of handling the general issues of distributed computing.

For sake of brevity, we will mention here only the Spark's features that are relevant to our scope. The main data structure used by Spark is *Resilient Distributed Dataset (RDD)*. An RDD is a read-only, partitioned collection of records. Spark's API allows the definition of custom functions in order to manipulate RDD when implementing our algorithm.

Two of the core Spark's functions, working on an RDD according to the the map-reduce paradigm, are the following: a) *mapPartitions*: RDD returned by mapPartitions is obtained by transforming each partition of the source RDD as specified by a user-defined function; b) *reduce*: RDDs are aggregated in pairs by using a user-defined function that must be commutative and associative in order to perform the reduction step in parallel.

As described in Section 3, the operations that CLUBS-P performs on data are commutative and associative, therefore we can safely adopt Spark for implementing our algorithm, that we call CLUBS*.

Since the computation of marginal distributions is the most expensive operation and the most interesting, from a technical point of view, in the following we provide in Algorithm 1 the details of its implementation using Spark.

Algorithm 1: *Marginal Distribution Computation.*

```
Input: D: RDD⟨Point⟩ representing points in a block $B$.
Output: Marginal distribution for $B$.
1: RDD⟨Map⟨Double, Integer⟩[]⟩ mc ←
   D.mapPartitions(new CMapper());
2: Map⟨Double, Integer⟩[] C ← ms. reduce(new
   CReducer());
3: RDD⟨Map⟨Double, Double[]⟩[]⟩ mls ←
   data.mapPartitions(new LSMapper());
4: Map⟨Double, Double[]⟩[] LS ← mls. reduce(new
   LSReducer());
5: return C, LS;
```

Lines 1–2 compute the *C* function over the input data, for every dimension. More specifically, line 1, computes this function for the data of each worker, through our object `CMapper`, which simply scans the data of the worker, updating a counter for each possible coordinate of each dimension. Then, line 2 aggregates the partial counts, using the object `CReducer`. The computation of *LS* functions is performed by lines 3–4. The object `LSMapper` is similar to `CMapper`, but instead of updating counters, it updates arrays representing the sum of points. The same holds for the object `LSReducer`.

[3]http://spark.apache.org/

In the following, we report a simple example that clarifies how map-reduce paradigm is applied by the algorithm.

Example 1. Consider a toy dataset consisting of 9 points partitioned over 2 nodes as follows::

$$part_1 = \{(4,4),(5,7),(5,8),(5,4),(6,4)\}$$

and

$$part_2 = \{(2,7),(2,5),(3,6),(5,7)\}$$

The results of the mapping operations (lines 1 and 3) for each node and each dimension are reported in Table 1.

Table 1: Results of the map operations.

part$_1$	dim 1	coord	4	5	6
		mc	1	3	1
		mls	(4, 4)	(15, 19)	(6, 4)
	dim 2	coord	4	7	8
		mc	3	1	1
		mls	(15, 12)	(5, 7)	(5, 8)
part$_2$	dim 1	coord	2	3	5
		mc	2	1	1
		mls	(4, 12)	(3, 6)	(5, 7)
	dim 2	coord	5	6	7
		mc	1	1	2
		mls	(2, 5)	(3, 6)	(7, 14)

For instance, the points in partition 1 that have coordinate of dimension 2 equal to 4 are the following: $(4,4)$, $(5,4)$, and $(6,4)$. Therefore, for the dimension 2 and coordinate 4 **mc** is 3, and **mls** is $(4,4)+(5,4)+(6,4) = (15,12)$.

The results of the reducing operations (lines 2 and 4) for each dimension are reported in Table 2.

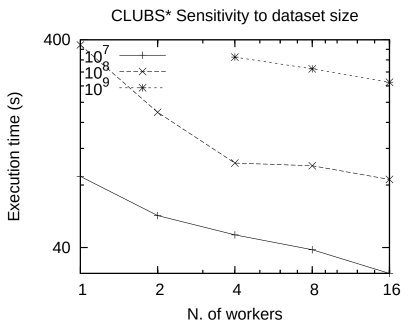
Table 2: Results of the reduce operations.

dim 1	coord	2	3	4	5	6
	C	2	1	1	4	1
	LS	(4, 12)	(3, 6)	(4, 4)	(20, 26)	(6, 4)
dim 2	coord	4	5	6	7	8
	C	3	1	1	3	1
	LS	(15, 12)	(5, 2)	(3, 6)	(12, 21)	(5, 8)

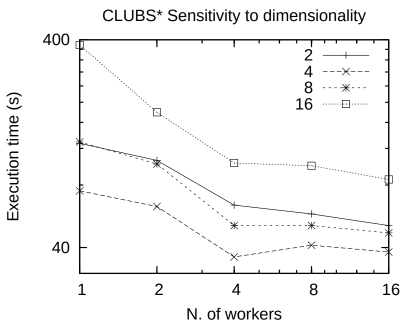
For instance, consider the coordinate 5 of dimension 1. **C** is obtained as $3+1=4$, and **LS** as $(15,19)+(5,7) = (20,26)$.

5 EXPERIMENTAL RESULTS

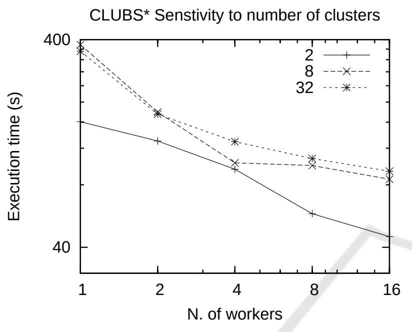
As mentioned above, CLUBS-P shares the ideas of CLUBS$^+$. Since the clustering obtained by CLUBS-P for a given data set is the same that obtained by



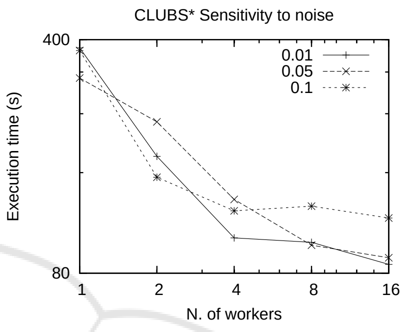
(a)



(b)



(c)



(d)

Figure 2: CLUBS* Execution Times vs number of workers varying dataset size (a), data dimensionality (b), number of clusters (c), and noise ratio (d).

CLUBS, we can say that the accuracy of CLUBS-P is the same as that of CLUBS. The latter has been proven to be better than that of existing algorithms (CLUBS,), and, thus, we do not report accuracy results here, for space limitation and because our goal is rather to prove the effectiveness of the parallelization of CLUBS$^+$ in order to apply it in the Big Data scenario. We tested our parallel implementation on several synthetic datasets obtained by means of an open source synthetic data generator[4], which generates data distributions where each cluster follows a possibly different gaussian distribution, while noise points are randomly added. We generated datasets with 10^7, 10^8 and 10^9 points. For each dataset size, we varied the dimensionality in the range [2..16] and the number of clusters in the range [2..32]. Finally, in order to test the robustness of our algorithm w.r.t. noise, we added a number of randomly distributed points ranging between 0 and 0.1 times the total number of points. Experiments were executed on a cluster having 16 computing machines (100GB RAM available each). As previously said, our implementations, according to *Reproducible Research (RR)* policy are publicly available[5]. We studied the running times obtained using 1, 2, 4, 8, or 16 workers[6], varying one data parameter at a time, while maintaining constant the other ones. The non-varying parameters, in each experiment were set as 10^8 points, 16 dimensions, 32 clusters, and 0.1 noise ratio.

In the following, we report the results obtained using *CLUBS**.

5.1 Evaluating CLUBS*

In this section, we report the performances obtained using CLUBS* in the same experimental setting, which are depicted in Figure 2. We found that the performances obtained by using the Spark-based implementation are less stable than expected, this is probably due to the fact that Spark uses some random shuffling of data which we can not control. Furthermore, with Spark assigning a given portion of the data set to each node is not achievable as the actual physical distribution of data among workers can not be controlled. In general, we found a good speedup for 2 and 4 workers, while the speedup is reduced when the number of workers is further increased. This is probably due to

[4]https://github.com/gmmazzeo/clugen

[5]https://github.com/gmmazzeo/clubspark

[6]We ran one worker per different machine of the cluster, thus, the number of workers and machines here are the same.

the overhead introduced by the Spark framework. In terms of sensitivity to the data parameters, from the experimental results we can observe that the speedup of CLUBS* is not affected by the data dimensionality and noise ratio (the absolute running time, instead, is affected by dimensionality, as expected). For the sensitivity to the number of clusters, the speedup is reduced when the number of clusters increases, because the divisive phase is the phase requiring the most network communication, and its duration increases with the number of clusters.

6 CONCLUSIONS

In this paper we discussed CLUBS-P, an algorithm for around-centroid clustering for Big Data. We evaluated a new implementation of CLUBS-P, in order to perform a kind of feasibility analysis w.r.t. the big data setting. The results obtained show a very good scalability of the algorithm.

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