String Patterns: From Single Clustering to Ensemble Methods and Validation

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Abstract. We address the problem of clustering of string patterns, in an Ensemble Methods perspective. In this approach different partitionings of the data are combined attempting to find a better and more robust partition. In this study we cover the different phases of this approach: from the generation of the partitions, *the clustering ensemble*, to the combination and validation of the combined result. For the generation we address, both different clustering algorithms (using both the *hierarchical agglomerative* concept and *partitional* approaches) and different similarity measures (*string matching*, *structural resemblance*). The focus of the paper is the concept of validation/selection of the final data partition. For that, an information-theoretic measure in conjunction with a variance analysis using bootstrapping is used to quantitatively measure the consistency between partitions and combined results and choose the best obtained result without the use of additional information. Experimental results on a real data set (contour images), show that this approach can be used to unsupervisedly choose the best partition amongst alternative solutions, as validated by measuring the consistency with the ground truth information.

1 Introduction

Let $D = \{s_1, s_2, \ldots, s_N\}$ be a set of N objects, and $s_i = \{s_1^i, \ldots, s_{L_i}^i\}$ be a sequence of length L_i symbols, defined over an alphabet Σ. Sequences clustering or string clustering is a particular form of clustering where objects are sequences of symbols, also known as strings.

Clustering algorithms for strings patterns are typically extensions of conventional clustering methods (assuming vector representations) to handle string descriptions, most of them by adopting a convenient measure of similarity between patterns [1, 2]. Clustering of string patterns has a broad range of applicability, such as: document image analysis (handwriting, maps, technical drawings strings); speech and one-dimensional signal analysis; DNA/genome sequencing and analysis; shape analysis; pattern-based speech recognition.

Choosing a particular clustering criteria, or induced similarity between given data points, is a difficult task, either in vector representations, either in string representations. Inspired on the work of sensor fusion and classifier combination, the most recent trend and best performing approach in cluster analysis is the so called "cluster combination" [3–5]. These methods attempt to find better and more robust partitioning of

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the data by combining the information of a set of N different partitions, the *clustering ensemble* - $\mathbb{P}$; formally, $\mathbb{P} = \{P^1, P^2, \ldots, P^i, \ldots, P^N\}$, where each partition, $P^i = \{C_1^i, C_2^i, \ldots, C_{k_i}^i\}$, has k_i clusters.

We build on a previous paper [6], where the clustering combination was evaluated in the context of string patterns. For the ensemble generation, different combinations of algorithms and proximity measures for string patterns are evaluated. The combination algorithms in this context can be used to combine different paradigms, as a multi-objective approach, attempting to find better and more robust partitioning of the data set, for example a distinct set of algorithms (K-Means clustering, Spectral Clustering, classical hierarchical methods) and/or different proximity measures.

The focus of this paper is the concept of validation/selection of the ”optimal” data partition. For that, and following [7], an information-theoretic measure, the concept of normalized mutual information, is used in conjunction with a variance analysis using bootstrapping, to quantitatively measure the consistency between partitions and the combined results and unsupervisely choose what is the best obtained result. The ground truth information, will be used to confirm the results and the performance of the different algorithms and ensembles.

Section 2 describes the ensemble methods approach in the context of String patterns; section 3 introduces the problem and possible solution for the validation of the solution; section 4 presents results and its discussion; finally section 5 draws conclusions.

2 Ensemble Methods for String Patterns

The approach of clustering combination, also known as Ensemble Methods, involves three different steps: the generation of the clustering ensemble, the combination of the clustering ensemble that results in the extraction of the combined data partition, P^*, and the validation of the result. Section 2.1 presents the production of the clustering ensemble for string patterns, involving different proximity measures and algorithms, and Section 2.2 presents the clustering combination methods.

2.1 Generation of the Clustering Ensemble

The clustering ensemble can be produced in many different ways, including: different algorithms; single algorithm with different parameter initializations or distinct parameter values; clustering different views/features of the data; manipulation of the data set, using techniques such as bootstrap or boosting.

Following previous work [6] the clustering ensemble for string patterns can be generated based on conventional clustering methods extended for string patterns by introducing proximity measures between strings [2].

Proximity Measures. The most common similarity measures belongs to the *string matching* paradigm and are based on String Editing Operations (SEO): substitution, maintenance, insertion or deletion of symbols. The Levensthein and the weighed Levensthein distances quantify the minimum number of operations required to transform a string s_i into another string s_j. Herein, we will adopt 0 cost to maintenance of a symbol and unitary cost for the remaining string editing operations. Moreover, different types of normalization are used, namely: the classical normalization by the string length (NSED); and the normalization by the length of the editing path – normalized string edit distance (NSEDL).

In a different paradigm, the *structural resemblance*, use grammars to model the cluster's structure, and rules of composition of clusters are assumed to reflect the similarity between patterns. Several approaches are described in the literature: Fu proposed a distance between strings based on the concept of error correcting parsing (ECP); Fred explored the notion of compressibility of sequences and algorithmic complexity using Solomonoff's code (SOLO); another approach by Fred, the ratio of decrease in grammar complexity (RDGC), is based on the idea that if two sentences are structurally similar, then their joint description is more similar than their isolated description due to sharing rules of symbol of composition. For details on how to compute these measures consult, for instance, [2] and the references therein.

Clustering Algorithms. Several clustering algorithms are addressed using both the partitional and hierarchical agglomerative approaches.

On the first approach, one of best well known and mostly used algorithm for clustering is the K-means algorithm. In order to apply it to string descriptions, we have adapted it, in order to be based on proximity measures described previously for string pairs. Moreover, the clustering prototypes are selected as the median string. A nearest neighbor approach, that we will refer as *Fu-NN*, was also explored, adopting as distance measure the string edit distance (SED). The nearest-neighbor rule is the basis for another algorithm, where clusters are modeled by grammars, but where sequences are compared, not directly with patterns previously included in clusters, but with the best matching elements in languages generated by the grammars inferred from clustered data. For grammatical inference we used the Crespi-reghizzi's method [2], without assuming *a priori* information. We will refer to this method as *FU-ECP*. In a different perspective the Spectral clustering algorithms [8] map the original data set into a different feature space based on the eigenvectors of an affinity matrix, a clustering method being applied to the new feature space. In order to extend the applicability of the method to string patterns, the definition of the affinity matrix is derived from the normalized string edit distance (NSEDL).

In the hierarchical perspective [9], we will explore the classical Single Link (SL), Complete Link (CL), Average Link (AL), Ward's Link(WL), and Centroid Based Link (Centroid) [9]. To convert the similarity measures defined above, generically referred as $S(s_1, s_2)$, into dissimilarity measures, we use:$d(s_1, s_2) = \max(\text{similarity}) - S(s_1, s_2)$

2.2 Clusterings Combination

Several combination methods have been proposed to obtain the combined solution, P^*, [3–5]. Fred and Jain proposed a method, the Evidence Accumulation Clustering (EAC), for finding consistent data partitions, where the combination of clustering ensemble is performed transforming partitions into a co-association matrix, which maps the coherent associations and represents a new similarity measure between patterns. To unsupervisely find the number of clusters, the lifetime method [3] can be used. Strehl and Gosh have formulated the clustering ensemble problem as an optimization problem based on the maximal average mutual information between the optimal combined clustering and the clustering ensemble. Three heuristics are presented to solve it, exploring graph theoretical concepts (CSPA, HGPA, MCLA). Topchy, Jain and Punch, proposed to solve the combination problem based on a probabilistic model of the consensus partition in the space of clusterings. In this paper we will be concentrated on the first approach - the EAC algorithm.

3 Clustering Validation

Different clustering algorithms lead in general to different partitions of the data set. The problem of evaluation/comparison of clustering results as well as deciding the number of clusters better fitting the data is fundamental in clustering analysis and it has been subject of many research efforts [9–12].In the context of clustering combination approaches the problem of clustering validation is still central. The selection/weighting of the best partitions or clusters of the clustering ensemble determines the performance of the clustering combination algorithms. Different approaches can be followed. The stability analysis, measuring the reproducibility of clustering solutions, either perturbing the data set or the clustering ensemble, offers an interesting solution [11, 13, 7]. We will focus in the stability analysis proposed in [7] where the robustness of the EAC algorithm was accessed by variance analysis, based on bootstrapping of the clustering ensemble.

3.1 Stability Analysis

The clustering ensemble $\mathbb{P}$ is perturbed using bootstrapping, producing B bootstrap versions of the clustering ensembles: $\mathbb{P}^B = \{\mathbb{P}^{b_1}, \ldots, \mathbb{P}^{b_i}, \ldots, \mathbb{P}^{bB}\}$, where $\mathbb{P}^{b_i}$ is a clustering ensemble that when combined will generate the combined data partition denoted by P^{*b_i}.

Using the normalized mutual information [7],defined as $NMI(P^a, P^b) = \frac{2I(P^a,P^b)}{H(P^a)+H(P^b)}$, and frequency counts as approximations for probabilities (in this case the percentage of shared patterns between partition) it is possible to define the average normalized mutual information between the k-cluster combined partitions and the bootstrap clustering ensembles, $\overline{NMI(P_b^{*k}, \mathbb{P}^b)}$, as:

$$\overline{NMI(P_b^{*k}, \mathbb{P}^b)} = \frac{1}{B}\sum_{i=1}^{B} NMI(P_{b_i}^{*k}, \mathbb{P}^{b_i}) \quad (1)$$

and the corresponding standard deviation, $std\{NMI(P_b^{*k}, \mathbb{P}^b)\}$ as:

$$std\{NMI(P_b^{*k}, \mathbb{P}^b)\} = \sqrt{\frac{1}{B-1}\sum_{i=1}^{B} (NMI(P_{b_i}^{*k}, \mathbb{P}^{b_i}) - \overline{NMI(P_b^{*k}, \mathbb{P}^b)})^2} \quad (2)$$

These two measures enable the verification of the consistency of the different combined partition $P_{b_i}^{*k}$ with each perturbed bootstrap version of the clustering ensemble $\mathbb{P}^{b_i}$.

The consistency of the result will also be evaluated in a different perspective, assessing if the combined results, $P_{b_i}^{*k}$, are consistent with each other. For that we define the normalized mutual information between $P_{b_i}^{*k}$ and $P_{b_j}^{*k}$, $\overline{NMI(P_{b_i}^{*k}, P_{b_j}^{*k})}$, as:

$$\overline{NMI(P_b^{*k}, P_b^{*k})} = \frac{1}{\binom{N}{2}} \sum_{i=1}^{B-1} \sum_{j=i+1}^{B} NMI(P_{b_i}^{*k}, P_{b_j}^{*k}) \tag{3}$$

For the measures presented in equations 1, 2, 3, similar definitions are used for defining $\overline{C_i(P_b^{*k}, \mathbb{P}^b)}$, $var\{C_i(P*_b^k, \mathbb{P}^b)\}$ and $\overline{C_i(P_b^{*k}, P_b^{*k})}$, where C_i represents the consistency index [14] that finds the best match between partitions, counting the percentage of agreement between the labelings.

4 Experimental Results and Discussion

To test the proposed approach we will follow previous work [6] and apply the stability analysis to the combination results resulting from the problem of unsupervised categorization of contour images of hardware tools, using string descriptions.

4.1 Data Set

The real data set is composed by 634 contour images of 15 types of hardware tools [15]: $t1$ to $t15$. As shown in Figure 1, some of the hardware tools have moving parts; different poses (open, closed and half open), leading to different shapes. When counting each pose as a distinct sub-class in the object type, we obtain a total of 24 different "objects". We will test the algorithms with this number of clusters.

String descriptions of object's shapes were obtained for each image, segmenting the object from the background, sampling the object boundary at 50 equally spaced points, and finally using 8-directional differential chain code [16] to describe the boundary.

Fig. 1. Data set. Typical samples of the database of images of hardware tools; string descriptions are used to represent the contours of images.

4.2 Single Clustering Results

Each of the clustering algorithms presented as basis for constructing the clustering ensemble was applied to the data set. Table 1 summarizes the obtained results, in terms

Table 1. $C_i(P, P^o)$ individual clustering results.

Algorithm	Similarity Measure/ Parameters	C_i	nc
NN-StoS-Fu	SEONL th=0.3	25.4	14
	SEO th=8	69.7	72
NN-ECP-Fu	SEO th=4	25.4	13
	SEO th=5	27.4	7
	SEON th=0.09	27.4	7
Kmeans	SEONL	48.3	15
	SEO	47.3	15
Hier-SL	SEONL	21.5	24
	SOLOM	15.9	24
	RDGC	24.3	24
	ECP	16.6	24
Hier-CL	SEONL	39.3	24
	SOLOM	54.9	24
	RDGC	42.4	24
	ECP	41.8	24
Hier-AL	SOLOM	57.3	24
Hier-WL	SEONE	**90.7**	24
	SOLOM	60.6	24
	RDGC	51.7	24
	ECP	55.2	24
Spectral	NSEDL σ=0.08	76.5	24
	NSEDL σ=0.16	67.4	24
	NSEDL σ=0.44	**82.6**	24

of the number of clusters (column ”nc”) in the data partition P and the corresponding consistency with the ground truth information, P^o, $C_i(P, P^o)$ (column ”C_i”).

These partitions, have very heterogeneous results, obtaining a minimum of 7 clusters using NN-ECP-Fu (with SEO and th=5), to the correct number of cluster and a consistency of 82.6% using spectral clustering algorithm, or 90.7% using the hierarchical Wards (WL) link.

4.3 Ensemble Methods Results and Validation

Using the combination techniques presented in section 2.2, we propose to combine the clustering ensemble, assuming known the number of clusters, K, (with the value 24), and using the lifetime criteria.

Following [6], two different experiments were conducted. The first, that we will call Heterogenous Ensemble, uses partitions produced by the different paradigms described above (with all the algorithms and proximity measures) in a total of 23 partitions. The second uses only the partitions obtained using the spectral clustering algorithm. For that, the followed approach consisted in fixing the number of clusters in each partition ($K = 24$) and varying the parameter σ within the interval $[0.08 : 0.02 : 0.5]$, where 0.02 corresponds to an increment, resulting on a total of 22 partitions.

Table 2 shows the obtained results of the combination of the two ensembles (Heterogeneous and Spectral Ensembles). The rows of the table represent the algorithms (SL, CL, AL, WL or Centroid) used in the extraction of the combined data partition from the co-association matrix. The columns represent the consistency index $C_i(P^*, P^o)$ and $C_i(P_b^{*k}, P^o)$, between the combined data partition and the ground truth, and the consistency index between the bootstrap versions of the clustering ensemble and the ground truth information (in terms of mean and standard deviation). Moreover the columns are divided in k-fixed and lifetime version of the combination method, representing the obtained result with fixed number of clusters (equal to the true number of clusters, K=24), and the with the lifetime criteria, that chooses the number of clusters that best suits the data. Notice that the consistency index, when the number of clusters is equal to the true number of clusters, is equal to the percentage of agreement (1- P_e).

Table 2. Results of the combination of Heterogeneous and Spectral clustering Ensembles in terms of the consistency index between the combined partition and the ground truth - $C_i(P^*, P^o)$ and between the bootstrap versions of the clustering ensemble and the ground truth - $C_i(P_b^{*k}, P^o)$.

Comb. Alg.	Heterogeneous						Spectral					
	k-fixed			life-time			k-fixed			life-time		
	Ci	Bootstrap		Ci	Bootstrap		Ci	Bootstrap		Ci	Bootstrap	
		$\overline{Ci}$	$std\{Ci\}$		$\overline{Ci}$	$std\{Ci\}$		$\overline{Ci}$	$std\{Ci\}$		$\overline{Ci}$	$std\{Ci\}$
EAC-SL	61.7	53.9	11.7	14.5	16.6	*3.3*	**83.8**	*76.9*	2.9	67.0	66.7	5.7
EAC-CL	73.3	63.7	9.8	**21.1**	19.2	14.5	69.9	71.2	3.0	79.5	70.6	2.6
EAC-AL	73.3	69.7	9.7	**21.1**	21.8	4.3	76.0	74.5	4.1	70.2	*71.2*	*3.3*
EAC-WL	**93.7**	*84.0*	*7.0*	14.5	16.1	6.7	80.4	81.1	*1.4*	**84.4**	64.4	28.0
EAC-Cent	77.0	68.9	13.5	**21.1**	*28.1*	16.5	79.7	75.9	3.9	76.3	73.8	6.0

The combination results have considerably higher results than the average performance obtained with the individual methods in the clustering ensemble (43.6% average consistency index). Moreover, it is worth noticing that the combination results outperform the best individual clustering results: the Heterogeneous clustering ensemble gives the best global performance (consistency index with the EAC-WL method -$C_i(P^*, P^o)$- of 93.7%). In the Spectral clustering ensemble the results are, as in the previous ensemble, better than the single clustering results. Due to reduced space, in rest of the paper only the heterogenous ensemble will be considered, since it obtains better results.

In terms of the different paradigms for the selection of the number of clusters in the combination method (using fixed-k or lifetime), in the heterogeneous ensemble the fixed-k outperformed the lifetime criteria, since the number of obtained clusters using this criteria was only 3 (or 2 in some cases).

To understand the bootstrap versions of each ensemble, in table 2, columns $\overline{C_i}$ and $std\{C_i\}$, represent the average and the standard deviation of the consistency between the combination of the bootstrap versions of the clustering ensemble, denoted by P_b^{*k}, and the ground truth P^o. As shown, the average consistency is different from the obtained with all the ensemble ($\mathbb{P}$), since these versions of the ensemble were obtained perturbing $\mathbb{P}$ via bootstrapping (i.e sampling with replacement). Moreover the standard deviation in some cases is very large, which manifest the variability of the bootstrapped ensembles.

The stability analysis will try to choose the best combined partition, or in another perspective, try to find *"How to choose the extraction method?"* and *"If we should use the k-fixed or lifetime criteria?"*

Table 3 present consistency results between the bootstrap versions of the clustering ensemble $\mathbb{P}^b$ and the obtained clustering combination results P_b^{*k}, in terms of $\overline{NMI(P_b^{*k}, \mathbb{P}^b)}$ (equation 1), $std\{NMI(P*_b^k, \mathbb{P}^b)\}$ (equation 2), and $\overline{C_i(P_b^{*k}, \mathbb{P}^b)}$, $std\{C_i(P*_b^k, \mathbb{P}^b)\}$, based on 100 bootstrap experiment (using the same number of partitions in each ensemble), for the heterogeneous and spectral ensembles respectively. Moreover it presents the consistency between the obtained combination results in the different bootstrap experiences, in terms of $\overline{NMI(P_b^{*k}, P_b^{*k})}$, $\overline{Ci(P_b^{*k}, P_b^{*k})}$.

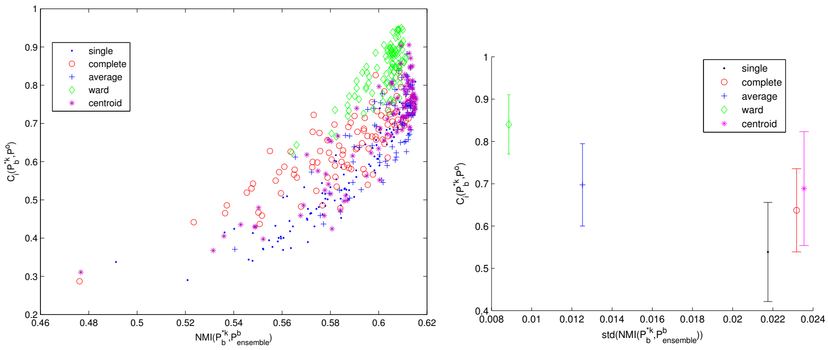
Table 3. Heterogeneous clustering ensemble - Column: $P_b^{*k}, \mathbb{P}^b$ represent the consistency between the bootstrap versions of the clustering ensemble $\mathbb{P}^b$ and the obtained clustering combination results P_b^{*k}, in terms of $\overline{NMI(P_b^{*k}, \mathbb{P}^b)}$, $std\{NMI(P*_b^k, \mathbb{P}^b)\}$, and $\overline{C_i(P_b^{*k}, \mathbb{P}^b)}$, $std\{C_i(P*_b^k, \mathbb{P}^b)\}$; Column: P_b^{*k}, P_b^{*k} represent the consistency between the obtained combination results in the different bootstrap experiences, in terms of $\overline{NMI(P_b^{*k}, P_b^{*k})}$, $\overline{Ci(P_b^{*k}, P_b^{*k})}$.

Comb. Alg.	fixed-k						life-time					
	$P_b^{*k}, \mathbb{P}^b$				P_b^{*k}, P_b^{*k}		$P_b^{*k}, \mathbb{P}^b$				P_b^{*k}, P_b^{*k}	
	NMI		C_i		NMI	C_i	NMI		C_i		NMI	C_i
	μ	std	μ	std			μ	std	μ	std		
EAC-SL	0.581	0.0217	**0.478**	0.0166	0.832	0.691	0.265	0.0872	0.441	**0.0058**	0.817	0.949
EAC-CL	0.586	0.0231	0.448	0.0185	0.815	0.652	0.240	0.2185	0.428	0.0059	0.417	0.713
EAC-AL	**0.605**	0.0125	0.463	**0.0106**	0.896	0.779	**0.392**	**0.0492**	**0.474**	0.0061	**0.890**	**0.950**
EAC-WL	0.603	**0.0088**	0.434	0.0126	**0.915**	**0.809**	0.309	0.0624	0.436	0.0060	0.572	0.848
EAC-Cent	0.599	0.0235	0.473	0.0149	0.859	0.731	0.408	0.1203	0.474	0.0059	0.639	0.761

Comparing the best obtained results (considering the ground truth information - table 2), for the fixed-k version was obtained with the EAC-WL (considering all the ensemble and also the bootstrap versions); and for the life-time approach the best results were obtained using the EAC-CL, EAC-AL and EAC-Cent (considering the bootstrap version the best was the EAC-Cent but with a high standard deviation, followed by the EAC-AL with a much lower standard deviation).

Following the average consistency between the combined results and the bootstrap ensembles - $\overline{NMI(P_b^{*k}, \mathbb{P}^b)}$ - the best partition is not always correctly chosen, the same happening with the $\overline{C_i(P_b^{*k}, \mathbb{P}^b)}$. The standard deviation measures of this consistency $std\{NMI(P*_b^k, \mathbb{P}^b)\}$ and $std\{C_i(P*_b^k, \mathbb{P}^b)\}$, are the more suitable for the selection of the best partition, choosing in the case of the NMI the best partitions (by other words best method). Moreover it leads to the choice of the k-fixed version (instead of the lifetime version) of the algorithm.

Following the other perspective, the consistency between the combination results (in the different bootstrap versions of the ensemble) - P_b^{*k} - in terms of $\overline{NMI(P_b^{*k}, P_b^{*k})}$, $\overline{Ci(P_b^{*k}, P_b^{*k})}$, the best partitions are selected. This measure can be considered a measure of reproducibility of clustering solutions, since with different clustering ensembles, obtained perturbing the original clustering ensemble, the different combined solutions



(a) Corr($NMI(P_b^{*k}, \mathbb{P}^b)$,$C_i(P_b^{*k}, P^o)$) (b) $std(NMI)$

Fig. 2. In both figure y-axis represent the consistency of the combined solutions with the ground truth - $C_i(P_b^{*k}, P^o)$. In the left figure the x-axis represents the NMI between the combined solutions and the ensembles $NMI(P_b^{*k}, \mathbb{P}^b)$; in the right figure the x-axis represent the standard deviation of this measure $std(NMI(P_b^{*k}, \mathbb{P}^b))$.

are compared. To understand the variability of the obtained solutions, Figure 2 presents the correlation between $C_i(P_{b_i}^{*k}, P^o)$ (y-axis) and $NMI(P_{b_i}^{*k}, \mathbb{P}^b)$ (x-axis).

It can be seen from the left figure, that the partitions with the best results (according with the ground truth information P^o - y-axis) are the partition with the symbol $\diamondsuit$ (in green), EAC-WL. The right figure, which represents the standard deviation of the combined results with the clustering ensembles, shows that was the chosen method.

Analyzing analogous correlations for consistency of the combined solutions, like, $\overline{NMI(P_b^{*k}, P_b^{*k})}$ lead to the same conclusions.

5 Conclusion

In this paper we focus the concept of validation/selection of the ”optimal” data partition in the Ensemble Methods perspective. The problem of clustering of string patterns was used as an example of application of this analysis. It consisted in a variance analysis using bootstrap to quantitatively measure the consistency between the partitions of the clustering ensemble and combined results and by the other hand the consistency between the obtained combination results in the different bootstrap experiments. These preliminary results show that the variance (standard deviation) of the consistency of the combined results with the clustering ensemble and the consistency between the combination results in the different bootstrap experiences lead to the choice of the most adequate solution. Further experiments are being conducted to further confirm this result.

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