Blanket Clusterer: A Tool for Automating the Clustering in Unsupervised Learning

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Abstract: We propose a generic hierarchical clustering algorithm - named Blanket Clusterer, which allows researchers to examine their data and verify the results gained from other machine learning techniques. We also integrate a three-dimensional visualization plugin that provides better understanding of the clustering results. We verify the tool on a specific use-case, i.e., measuring the clustering techniques performances on a textual dataset based solely on ICD-9 descriptions encoded using the Word2Vec distributed representations. The verification shows that Blanket Clusterer provides an efficient pipeline for evaluating and interpreting the most frequently used clustering methods in unsupervised learning.

1 INTRODUCTION

Clustering is one of the most popular machine learning techniques regarding unsupervised learning methods. The idea behind them is to use mathematical equations to successfully divide the dataset into subsets. These algorithms allow the user to automatically divide the set into subsets, perchance gaining previously unknown facts about it (Bhardwaj et al., 2019). The effort to execute the clustering algorithms and determine the best one is often a time-consuming and exhaustive task that depends on the dataset format and characteristics. This paper presents a tool that encompasses multiple clustering techniques, named Blanket Clusterer. Blanket Clusterer, in terms of problems revolving around clustering data, automates the complex process of dataset preparation, execution, and evaluation of different families of clustering algorithms based on dataset metadata and algorithm requirements. Furthermore, it implements advanced 3D visualization plots to better interpret the algorithms’ results and aid the algorithms assessment and verification process. Blanket Clusterer currently incorporates multiple clustering algorithms which we discuss in this paper. They vary from bottom-up to top-down approaches, from hierarchical to non-hierarchical algorithms. Furthermore, regarding the hierarchy segment of our algorithm, due to the fact that not all clustering algorithms are hierarchical algorithms and our use-case has a dataset which needs hierarchy, we implement a custom hierarchical algorithm, which divides the set into subsets, thus implementing this feature in clustering algorithms which did not have it.

In this study, we perform verification of the clustering tool on a specific use-case scenario. All claims submitted by physicians to the Medical Services Plan (MSP) must include a diagnostic code. This information allows MSP to verify claims and generate statistics about causes of illness and death. The International Classification of Disease (ICD) coding system divides diseases and health conditions into similar categories based on body systems and health conditions. More specifically, ICD-9 diagnostic codes are based on the ninth revision of the coding standard. The ICD-9 codes are organized into 19 chapters, and a specific code range identifies each chapter. Each diagnosis is presented by ICD-9 code and description. First, we leverage these textual descriptions to build a dataset that we are using to verify the tool we propose. Next, we use Word2Vec to encode these descriptions into a distributed vector representation. The results, the sequence of real-valued vectors, are given as input to our Blanket Clusterer tool to perform clustering using the implemented clustering algorithms. Finally,
we assess the category label for each diagnosis obtained from the clustering algorithms’ output by comparing it to the ICD-9 chapter, thus measuring their effectiveness to categorize the texts using only the diagnosis descriptions.

Lastly, we develop a three-dimensional visualization tool, which works with the results in visually representing them for ease of use. The main tool which was used for the hierarchical representation is CarrotSearch’s FoamTree\textsuperscript{1}, as described in Section 3 Blanket Clusterer.

As a short summary of our work, we:

- propose a generic hierarchical clustering module that integrates the most common used clustering algorithms;
- provide three-dimensional representation of the obtained clusters, with various color-coded values, for easier interpretation of the results;
- provide statistical information about performance (time, number of clusters) related to the different types of covered clustering algorithms, while also offering a foundation for future implementations of new clustering algorithms - either by implementing an already existing one, or building a brand new one from scratch, as long as it handles the specific object type which we already cover in the algorithm.
- validate clustering results with silhouette scores for each algorithm used.

The Blanket Clusterer tool and code is available on:

- Docker, though their DockerHub library, on docker.hub/kbogdanoski/blanket-clusterer
- GitHub, available at git.com/Blanket-Clusterer

\section{RELATED WORK}

We previously stated that Blanket Clusterer is an algorithm which covers different clustering algorithms, hence the word "blanket" in the name. K-Means is one of the algorithms which is being broadly used in various Machine learning studies(Govender and Sivakumar, 2020). K-Means is an algorithm which exists for at least 60 years and although there have been a couple of algorithms which have had a proof of concept after it, k-means has remained as one of the most widely used algorithms due to its simplicity, ease of implementation and efficiency(Jian, 2009)(Govender and Sivakumar, 2020). Aside from work with datasets extracted from textual information, through a natural language processing technique, k-means has shown that it does not make any difference when it comes to using datasets when they come from different industries, such as using data in studies related to spatial-temporal characteristics of air pollution, pollutant behavior in terms of space and so on(Govender and Sivakumar, 2020). De facto, the authors of the paper(Govender and Sivakumar, 2020), focus on the problem with applying k-means and hierarchical clustering techniques for analysis of air pollution, since clustering has been widely applied to atmospheric science data, climate and meteorological data.

Clustering algorithms work with mathematical equations, thus they need numerical values for the calculations. Although words, sentences, can be transformed into numeric vectors, while at the same time containing much valuable information, the same can be said with processing images, as they, on the bottom side, are an array of numerical values representing the pixels and position of them. Re-identification is a sub-task in the field of image processing problems, as the main goal is to match pictures of the same person that appears in different cameras, commonly used as a tool in the identification of pedestrian crossings around the world in the feat to identify pedestrian information(Zeng et al., 2020), allowing the officials to maintain control without being present at the said intersection.

The authors in (Glielmo et al., 2021) propose an overview of all algorithms currently used to extract simplified models from molecular simulations to understand the simulated systems on a physical level. More precisely, they discuss feature representation of molecular systems and present state-of-the-art algorithms, divided in five sections: dimensional reduction, density estimation and clustering, and kinetic models. Figure 1 shows possible steps that can be performed to analyze data from a molecular simulation with an indication of the particular section in which they are used - Density estimation and Clustering.

According to the research done with the paper "Combining hierarchical clustering algorithms using the PCA method"(Jafarzadegan et al., 2019), it was confirmed that the performance of the various unsupervised learning techniques, specifically clustering and classification designs, depends on the problem at hand, as well as the pertinent method used to solve said problem. Additionally, using the same, or similar, method for contrasting problems, might and most likely will, produce unreliable results. For this reason, Blanket Clusterer allows the researchers to try out different types of clustering algorithms, in an ef-

\textsuperscript{1}FoamTree is available at https://www.carrotsearch.com/foamtree/
Unsupervised learning methods for molecular simulation. Effort to find the best one, while testing out different possibilities at the same time.

Even though a clustering algorithm is selected for the task at hand, researchers still might not be pleased with the results. Further optimization is possible through the use of Principal Component Analysis - PCA, as shown in the research paper: "Optimization of fuzzy c-means clustering algorithm with combination of minkowski and chebyshev distance using principal component analysis" (Surono and Putri, 2021), where it was shown that reducing the number of dimensions for each entry in the dataset, while using PCA as a technique, the clustering accuracy obtained had an accuracy score of 1.6468 (Surono and Putri, 2021). PCA, or principal component analysis, is an analysis method which aims to transform a high-dimensional dataset into a low-dimensional space, while not losing any of the features which are important to the knowledge of the model. PCA uses algebraic equations to reduce dimensions that are interconnected with other dimensions within the dataset, into new data with unrelated dimensions named principal components (Farjo et al., 2013).

Aside from using PCA as a tool to optimize custom clustering algorithms, it can also be used in already-known algorithms. As shown by the research of Abdulhafedh (Abdulhafedh, 2021), using PCA alongside the K-Means clustering algorithm in the aim to divide a dataset containing customers into segments, so plausible marketing strategies may be used for the customers with whom the possibility of them accepting the offer, is greater than before.

We mention PCA as it is a valuable tool in unsupervised learning techniques, as it is a feature which will be developed to work alongside Blanket Clusterer, to further provide assistance and recommendations to the researchers who do use this tool.

In recent years, data scientists have become very hard to find, due to the high demand. AutoML, similar to Blanket Clusterer, is a tool which aims to remove the need of having a data scientist to analyse, preprocess, process, extract knowledge from a dataset, with providing a tool to allow other users, such as domain experts, to automatically create machine learning applications, without the prerequisite of having statistical and machine learning knowledge (He et al., 2021). As shown in Figure 2, AutoML extracts features from the dataset, it generates a model for said dataset, and estimates the model, prior to providing it to the user. In contrast to AutoML which provides tools for supervised learning, using the benefits of techniques such as Convolutional Neuron Networks (CNNs), and Recurrent Neural Networks (RNNs), Blanket Clusterer is a tool which handles tasks related to unsupervised learning, mainly clustering algorithms for unlabeled and/or labeled data, using the benefits of the simple to understand techniques, their efficiency and efficacy (as shown in Figure 3). There are various implementations of AutoML, including Google’s Cloud AutoML.

EfficientDet is a tool in the AutoML segment (Tan et al., 2020), which aims to increase the efficiency and scalability, while also providing optimizations for further improvement. As an important note EfficientDet’s algorithm operates in supervised learning manor, especially object detection in provided datasets. Blanket Clusterer on the other hand, provides results for whatever task, as long as the dataset conforms to the requirements of the tool in terms of the format. GIT (Gao et al., 2021) is another clustering algorithm, based on graph clustering which aims to increase the performance related to graph clustering. This contrasts our tool which can handle datasets from different sources, as previously stated.

HypHC (Chami et al., 2020) is a hierarchical clustering algorithm, with a goal to compare different algorithms, measure their quality and explain their success or failure, similar to our tool. The main difference between these two algorithms, is that HypHC utilizes the discrete cost function over space proposed by Dasgrupta (Dasgupta, 2016), while Blanket Clusterer does not, in its current state.
3 BLANKET CLUSTERER

3.1 Goal

Blanket Clusterer is a Python module which aims to provide a straightforward generic hierarchical clustering algorithm, alongside a clean 3D\(^2\) visualization, to better understand the received results.

The tool integrates the most commonly used clustering algorithms in one place:

- K-Means
- Agglomerative
- Birch
- DBSCAN

As an important side note, DBSCAN due to its implementation, does not provide the preferred results, compared to the other algorithms, thus this algorithm was not part of our testing and validation segment.

Additionally, Blanket Clusterer adds another level of functionality in allowing to hierarchically cluster data with said algorithms, as well as adding a visualization functionality, using CarrotSearch’s FoamTree\(^\text{TM}\) library, and measuring their performance through Silhouette scores.

3.2 Implementation

As previously stated, Blanket Clusterer works with other types of clustering algorithms. Aside from using these algorithms, it also eases the process in using them, with automating the whole process. Additionally, Blanket Clusterer provides a three-dimensional visualization of the results and provides a Silhouette metric of the clustering results for each algorithm.

The pipeline (shown in Figure 5) implemented in the Blanket Clusterer, consists of multiple steps. All of the classes are built upon a predefined class (Generic Clusterer, as shown in Figure 4), in which we have defined those methods that are needed for each algorithm.

![Generic Clusterer classes.](image)

Figure 4: Blanket Clusterer classes.

As previously stated, the execution pipeline of the algorithm is shown in Figure 5. The pipeline starts with the constructor, or the \_init\_() method. This method sets up the object which will be used to cluster the data. It fills the necessary attributes with the needed data.

As we initialize the Object, when creating a new variable, the constructor is called. After creating the object, we need only to call the method clusterize() which will inherently call other methods in the class.

The first method in the pipeline after clusterize() is the extract vectors() which will extract the vectors into the required format. The vectors are stored in a dictionary in a key-value format.

After extracting the vectors, we extract the keys so we can have them in a dictionary, with the extract names() method. This method is needed for evaluation purposes to compare the cluster predictions to the ground-truth clusters.

Next, we need to extract the group names, if provided, using the extract group names() method. This is quite similar to the name extraction process, but we will talk about it more in the next section.

The embeddings, names and group-names are not the only attributes necessary for our algorithm. We also need to extract the number of times a key is seen in the cluster and in which group it belongs to. Using the extract nums count() does that for us, and this is

\(^{2}3D\) - Three dimensional representation
needed for a better presentation of the results.

Alongside the number of times a code occurs in a cluster, are the coverage values, which are extracted with `extract_coverages()`). Those coverage values provide the color for our entities in the cluster, and the whole cluster overall. This is also not necessary, just like the group-names and the number of occurrences. The color is produced with a simple mathematical equation, because the color format is HSL\(^3\), we can divide the number 360 by the number of groups there are. With this simple math equation, we give a certain group, a certain color, which in return provides us with a better visualization in the end.

Until now, we have extracted the vectors in a dictionary, and the code they represent in the key position of the dictionary, but the algorithms need numerical arrays to operate. The method `extract_vectors.as_array()` does that for us, and stores the numerical values as arrays, making them ready for clustering.

After all these methods, comes the `run()` method, which checks if everything was okay up until this point, and starts the process of hierarchically clustering the data. If everything passes okay to this point and all the data entered was valid, the process should provide results without any setbacks.

### 3.3.1 Hierarchical Algorithm

The crucial part of our tool is having hierarchical result of the datasets. Our hierarchical algorithm is custom made, displayed with the pseudo code shown in Figure 6.

The pseudo code is straight-forward. Initially we give the tool a huge cluster of data. The tool then clusters the bigger cluster into smaller sub-clusters (the number of sub-clusters - \( N \), is provided by the user). Afterwards, for each sub-cluster, there is a simple check: If the total number of elements in the cluster \( X \), does not exceed the maximum allowed number of elements in a cluster \( M \), clustering for the current level is completed. Otherwise if \( X \) is greater than \( M \), another check is needed to see how big the difference is. If \( X \) is greater than \( M \) squared \((M^2)\), then the cluster is divided into sub-clusters with \( N \) elements in each one, otherwise the cluster is divided into sub-clusters with \( \frac{N}{M} \) elements in the cluster.

```plaintext
1. Cluster the current cluster into \( N \) sub-clusters
2. For each sub-cluster in the result:
   - if (total number of elements in sub-cluster \( K \) is greater than the maximum number of elements \( M \) then:
     i) If \( X > M \), then
       - re-cluster the current cluster with \( N \) sub-clusters
     ii) For each sub-cluster
         - re-cluster the current cluster with \( \frac{X}{N} \) elements in the cluster
   else Stop clustering
```

Figure 6: Hierarchical algorithm pseudo-code.

### 4 USE-CASE EVALUATION SCENARIO

#### 4.1 Dataset

To validate Blanket Clusterer, a specially designed dataset comprised with ICD-9 descriptions of the diagnoses is used. The Word2Vec word vectors are used for encoding these descriptions. We took the word embeddings from Word2Vec and applied clustering techniques with our tool.

The final input for the Blanket Clusterer is composed of a dictionary, whose key is the ICD-9 code, and value is the diagnosis description represented as a list of word vectors, as shown in Table 1. We use Blanket Clusterer to cluster the vectors (shown in Table 2), hierarchically and validate the results afterward.

```
<table>
<thead>
<tr>
<th>Key</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>001</td>
<td>[0.11, 0.22, ..., 0.99]</td>
</tr>
<tr>
<td>002</td>
<td>[0.22, 0.33, ..., 0.88]</td>
</tr>
<tr>
<td></td>
<td>...</td>
</tr>
<tr>
<td>E999</td>
<td>[0.99, 0.99, ..., 0.99]</td>
</tr>
</tbody>
</table>
```

To better understand the clustering results, aside from using the model’s embeddings, we also provide a dataset consisting of human readable names of the ICD-9 codes, so Blanket Clusterer can hierarchically name the clusters accordingly. This allows us to further validate our tool, with comparing the performance. As shown in Table 2, each ICD-9 code corre-
sponds to a specific human readable name.

Table 2: Key - Value of names.
<table>
<thead>
<tr>
<th>Key</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>001</td>
<td>Cholera</td>
</tr>
<tr>
<td>004</td>
<td>Shigellosis</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>E999</td>
<td>Late effect of injury due to war operations and terrorism</td>
</tr>
</tbody>
</table>

Similar to the previous dataset, the second dataset, aside from our Word2Vec model and key-names dataset, consists of specific names depicting groups of ICD-9 codes, as shown in Table 3. This dataset contains information about sets of ICD-9 codes, corresponding to a certain group in the ICD-9 naming scheme.

Table 3: Key - Value of group-names.
<table>
<thead>
<tr>
<th>Key</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>001-009</td>
<td>Intestinal Infectious Diseases</td>
</tr>
<tr>
<td>010-018</td>
<td>Tuberculosis</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>E990-E999</td>
<td>Injury Resulting From Operations Of War</td>
</tr>
</tbody>
</table>

After providing the algorithm with the datasets, we review the results through the 3D representation tool which we implement in Blanket Clusterer, and through the Silhouette score.

4.2 Results

All tests were done with the following parameters (shown in Table 4):

Table 4: Parameters and values used in test run.
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of diagnoses</td>
<td>16,728</td>
</tr>
<tr>
<td>Number of clusters in a hierarchy level</td>
<td>19</td>
</tr>
<tr>
<td>Number of entities in a cluster</td>
<td>19</td>
</tr>
<tr>
<td>Maximum depth of hierarchy</td>
<td>6</td>
</tr>
</tbody>
</table>

4.2.1 Visualization

As shown in Figure 8 and Figure 9, there is a clear distinction between the results, regarding the color-coding of clusters. As previously stated, in the results shown in Fig. 9, with the test run we provided a dataset containing the names of groups with codes, hence each color represents a certain group of ICD-9 codes. Each color represents one specific chapter of the ICD-9 taxonomy, thus proving that the algorithm has successfully clustered the diagnoses to a particular chapter as declared in the ICD-9 taxonomy.

Aside from the color, the names of the main clusters also vary between the figures. Because we have a custom naming scheme for them. It is easier to understand and validate the results when all features, which Blanket Clusterer provides, are used.

Figure 8: Visualization without group-names.

Figure 9: Visualization with group-names.

4.2.2 Cross-algorithm Performance

We measured the cross-algorithm performance through the Silhouette score (Shahapure and Nicholas, 2020), which represents the overall quality of the clusters in terms of the similarity between the vectors in each cluster, including the hierarchical groups of clusters. The score ranges from 0 to 1, where:

- 0 means the elements between the clusters are similar to one another
- 1 means that the elements between the clusters are very well separated

Having a higher score, means the clustering algorithm successfully separates the elements into clusters, filled with similar values, while the opposite is a fact with lower scores.

The Silhouette algorithm, since we have a hierarchical clustering tool, was calculated hierarchically and comparatively between clusters, meaning elements belonging to a certain cluster on certain level in the hierarchy are compared to elements belonging...
to the other clusters on the same level in the hierarchy. This score showed that the clusters, although not perfect, are close to the groups provided with the ICD-9 standard.

Table 5: Overall Silhouette score by algorithm.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Silhouette score</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Means</td>
<td>0.7151</td>
</tr>
<tr>
<td>Birch</td>
<td>0.7059</td>
</tr>
<tr>
<td>Agglomerative</td>
<td>0.7257</td>
</tr>
</tbody>
</table>

The amount of clusters generated is shown in Table 6, and for each algorithm, the average Silhouette score is depicted by Table 5.

Table 6: Total number of clusters.

<table>
<thead>
<tr>
<th>Algorithm</th>
<th>Total number of clusters</th>
</tr>
</thead>
<tbody>
<tr>
<td>K-Means</td>
<td>2200</td>
</tr>
<tr>
<td>Birch</td>
<td>1895</td>
</tr>
<tr>
<td>Agglomerative</td>
<td>2160</td>
</tr>
</tbody>
</table>

As shown by our tests, Agglomerative clustering outperforms the other algorithms, K-Means by 1%, while Birch by 2%. As previously stated, even though DBSCAN can be used in the algorithm, the hierarchical aspect could not be used, due to its implementation. Ergo, this clustering algorithm is not part of the research.

5 CONCLUSION

This paper presents a novel tool named Blanket Clusterer, which unifies the most widely used clustering techniques in Machine Learning and facilitates their application to various numeric representations of texts, sounds, and videos. We successfully validated Blanket Clusterer by a dataset comprised of ICD-9 descriptions. The tool proved its efficiency in applying different clustering methods to the dataset and providing a detailed report. Furthermore, Blanket Clusterer provides a valuable interpretation of the best clustering results through a three-dimensional visualization plot. In our specific use-case, the Agglomerative clustering offers the best results, compared to the other algorithms, with a higher Silhouette score than the rest, with a value of 0.7257. This research proves that Blanket Clusterer is a valuable tool for measuring the efficiency of clustering algorithms on a specific task. Lastly, the code and its interfaces are publicly available and open-sourced, thus incentivizing researchers to further enhance and expand its functionalities.

REFERENCES


