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Role of Metrics in Medical Image Analysis based on Unsupervised Machine Learning

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Background and Purpose: Our study addresses one of the complex aspects of machine learning techniques, namely the unsupervised machine learning applied to medical image analysis. While unsupervised learning has many benefits, there exists a main challenge that due to the fact that the result obtaining might be less accurate as input data is not labelled, and algorithms do not know the exact output in advance. Consequently, in unsupervised learning problems, several aspects must be taken into account for the validation of the algorithm results. These were the integration of measures in unsupervised learning algorithms is important. Metrics play multiple roles such as in image analysis, and in the judgment of the algorithm's performance. On the one hand, the paper describes a methodology for building an unsupervised machine learning with an application related to the analysis and diagnosis of medical images. On the other hand, it highlights the role of metrics and their mathematical properties in solving problems through unsupervised machine learning.

Methods: Considering the objectives of the medical image analysis such as to detect patterns on the image and to guide the diagnosis, we focus our interests on the unsupervised machine learning, specifically the clustering approach based the centroid and density models. These two models allow the image analysis and classification. Furthermore, we considered that classification can be done by attribution criteria such as object semantic and similarity criteria.

Results: We have demonstrated the application of unsupervised learning for medical image analysis and diagnosis. Our model was tested on 40 different images of samples. The accuracy in our unsupervised machine learning means detection and correct classification of all necessary objects in a single image.

Conclusions: Asking the machine to make a suitable grouping of the objects of an image in classes without human intervention by algorithms, this is the goal of unsupervised machine learning. To achieve this challenge, metrics play an important role. We built the formal model based on a set of rules and functions that can analyse and classifies objects' image in classes. Our model as the benefit to be used for semi-supervised machine learning co-clustering applications. This can make it easier to label a large volume of data.

Keywords: Unsupervised machine learning, classification, clustering, metrics, image analysis.

1 Introduction

Since a long time, without scientific instruments and materials the discovery and understanding of microorganisms and organisms would have been utopian. Microorganisms, in the world, are characterized by beings invisible to the human eye and which cause many health concerns for the latter, such as microbes. Seeing organisms in the body, finding any abnormality is of a great importance for human health and life expectancy.

A biomedical image is the materialization in the form of images of anatomical or functional information in vivo of parts (organs, tissues, cells) of the human body, as well as the data extracted or derived from these images. But it can also be an image obtained ex vivo (such as for example microscopy images of samples obtained by biopsy for pathological anatomy or by thick film for parasitological analysis).

The medical image corresponds to the localized measurement of a physical signal of an object or objects in space, generally in two dimensions (2D) or in three dimensions (3D). In radiologic imaging, "*the*

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intervention of the radiologist is to explore a field of view which can be either the whole object or a part of the object" [1]. As the same in microscopic analysis, the lab tech and the biologist observes different parasite forms. Doing this job manually with an *"explosion of medical data can lead to an upheaval in the workload of radiologists, limiting the time spent with the patient and increasing the rate of error in interpretation"* [2].

Thus, under the conditions of precision and real-time medicine in accordance with [3], "*the potential of medical image analysis by artificial intelligence (AI) is immense to provide faster and more reliable diagnosis to patients"*. Furthermore, "*most of the concepts used in AI come from or are inspired by neuroscience research. The concept of neural network, or layers of neurons, comes from the understanding of the organization of the cerebral cortex, particularly the visual cortex of the cat. Indeed vision is not a holistic phenomenon where visual integration would be done globally, but a hierarchical, sequential system, within which each visual region is responsible for a segmental analysis of the characteristics of the image, edge, intensity, pattern, colors, and movement*" [4].

The collaboration of imaging professionals with artificial intelligence and machine learning technologies is becoming more and more frequent, even if it is not yet very present in some health systems in southern Saharan countries. And it is quite obvious that imagists are concerned about the quality of the automatic image analysis and diagnosis provided.

As stated in [5], "*creating strong evidence for the usefulness of ML models in clinical settings is an involved process. It requires a thorough understanding of the properties of the model itself and its performance*."

Our study addresses one of the complex aspects of machine learning techniques, namely the unsupervised machine learning applied to medical image analysis. While unsupervised learning has many benefits, there exists a main challenge that due to the fact that the result obtaining might be less accurate as input data is not labelled, and algorithms do not know the exact output in advance. Consequently, in unsupervised learning problems, several aspects must be taken into account for the validation of the algorithm results. These were the integration of measures in unsupervised learning algorithms is important. Metrics play multiple roles such as in image analysis, and in the judgment of the algorithm's performance.

On the one hand, this article describes a methodology for building an unsupervised machine learning with an application related to the analysis and diagnosis of medical images. On the other hand, the article highlights the role of metrics and their mathematical properties in solving problems through unsupervised machine learning.

2 Materials and methods

There are different types of machine learning: supervised, unsupervised, and reinforcement. In particular our study focused on unsupervised learning that derive insights directly from the data itself and have capability to uncover patterns in an unlabelled dataset.

Since it is about the analysis of images, specifically of 2 dimensions, it is therefore assumed a geometric surface and a domain containing objects. Objects are characterized by their shape or structure, by their position in the surface and also by appearance. Moreover, the rules for assembling objects in the domain are based on notions such as inclusion and proximity. This is why having an image analyzed by a machine, in general, requires the integration of geometric measurements.

As mentioned earlier in the introduction, the following is a methodology of building an unsupervised machine learning for an application a medical image analysis and an automatic diagnosis. Behind, there are descriptions of metrics to be used which demonstrate their roles. The work published in the following articles, [6] [7] [8] [9], constitutes a basic part of our research.

And in the aspect of testing the performance of our system, we resorted to other metrics such as those of the Kolmogorov-Smirnov test [10] and normalized cross-correlation [11].

2.1 Unsupervised Machine Learning

The unsupervised machine learning model [12] has often three steps namely: data collection, building and training model, and at least the evaluation. In general, unsupervised machine learning has two model: clustering algorithm and association algorithm.

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The present study refers mainly to clustering. The clustering [13] [14] technique aims to discover meaningful structure or to identify patterns in the input data and then put it in a specific class/cluster.

2.1.1 Clustering Model

The clustering analysis of an image aims is to identify which of a set of categories a pattern belongs to. Moreover, a clustering algorithm maps input data to a category which can be a disease. The use of maths or metrics in clustering algorithms is mandatory to perform the clustering problem.

The theories presented in [15] on clustering models fixed our issues. Considering the objectives of the analysis of a medical image such as to detect patterns on the image and to guide the diagnosis, we pay attention to two models namely: the centroid and density models.

a) Centroid Model

K-means algorithm is one of the centroid based clustering algorithms. As stated in [16], "*when the data space X is R^D and using Euclidean distance, we can represent each cluster by the point in data space that is the average of the data assigned to it. Since each cluster is represented by an average, this approach is called K-Means*".

We illustrate the problem in the following way.

As the image space is *X*. Let consider *X* be R^D. Moreover, the data set is $\{x_n\}_{n=1}^{N}$. In this set of data belonging to the space *X*, the algorithm searches for points or elements having a particular interest based on a given invariant or threshold. These different points of interest are considered as centroids.

Let data (x_i), $i=1, 2, \ldots, n$, measured on *n* independent observations. It comes that $d_{ii'}$, denotes the distance between observations *i* and *i'*. Ultimately, the Euclidean distance *d* is:

$$d = \sqrt{\sum_{i=1}^{n} (x_i - x_{i'})^2} \quad (1)$$

The algorithm should also, in the meantime, calculate an area of interest around the central point using density model. This should make it easier to calculate the distance around the centroid.

From this point of view and in the medical context, the designer of the machine learning is supposed to define beforehand the clusters which correspond, for example, to a pathology. *K* represents the number of clusters *C.* Thus it is possible to determine *n-K* clusters as prototypes. But due to letting the machine has a self-learning, we formalize *K* in the following open interval (*n-K* to *m-K*); *m-K* is a discovered prototype.

$$K = [\![1..n \quad \Longrightarrow \quad K = \begin{cases} c_{1=k_1} \\ \ldots \\ c_m = k_m \end{cases}$$

b) Density Model

Intuitively, the density of a given surface is understood as the fraction of the total number of elements over the size of the surface. As stated in [17] [18] [19], the usual density measurement model will have to involve two ingredients, namely a local density estimate at each point and a connection between objects. From the above, we formulate:

$$\rho_i = \sum_j X(d_{ij} - d_c)$$
$$X(x) = \begin{cases} 1, x < 0 \\ 0, x \geq 0 \end{cases} \quad (2)$$

where ρ_i is a local density, d_{ij} is the Euclidean distance between data point *i* and data point *j*, and d_c is the cutoff distance; χ is the weighting function for estimating the influence of a neighboring point.

2.1.2 Classification

Image classification is a very common task in healthcare computer vision problems. And Machine learning are frequently employed for classification.

Let a class be defined by a set of properties which are both necessary and sufficient for membership in the class. Starting from the principle that the descriptions of the objects to be classified, whatever the initial format, are translated into geometric representations where each object is associated with characteristics. Thus, we ask ourselves the question: knowing, for a given object *o*, these characteristics $f(o_i)$, can we determine the class c_i to which this *o* belongs?

Knowing that unsupervised learning problems the labels in the input data are typically unknown.

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Two methods presented above, can help to solve the problem, since they are used to cluster the data together and to provide information about the structure of the data. This is the class identification.

Furthermore, classification can be done by attribution criteria such as object semantic and similarity criteria.

a) Object Semantic

The first criteria is the domain-object relationship. An object corresponds to a series of domains, with more or less features or characteristics defined as an object semantic.

$$f(o_i) = \{f_i : f_i \in D_j^{k+1}\} \tag{3}$$

b) Similarity

The 2nd criteria is a similarity. A classification always involves much more arbitrariness than does a representation of data in a geometric continuum, with, as coordinates, the factors extracted by a suitable analysis. Despite the fact that once the machine has discovered the semantic values of the object, it can proceed to a comparison with the theoretical models and prototypes of the intrinsic classes of the machine.

In our model uses a numerical value called the discrimination threshold. This threshold determines attribution of an object to a class. Let formalize below the rule of attribution:

$$S = \begin{cases} if\ 0 \rightarrow \text{"Similar"} \\ elseif\ [1..10] \rightarrow \text{"Bit similar"} \\ elseif > 10 \rightarrow \text{"Different"} \end{cases} \tag{4}$$

where *S* is the percentage of similarity; If two images are similar, their similarity percentage will equal to 90-100%, that is <10, but if different usually >30, that is [0-70%].

3 Results

We have demonstrated the application of unsupervised learning for image analysis for medical diagnosis. This application was produced as part of a project "Virtual Community of Healthcare Facilities" and relates to a medical decision support system for the management of malaria [20] [21].

3.1 Experimentation of Unsupervised Machine Learning for Automatic Diagnosis of Plasmodium

3.1.1 Data Collection

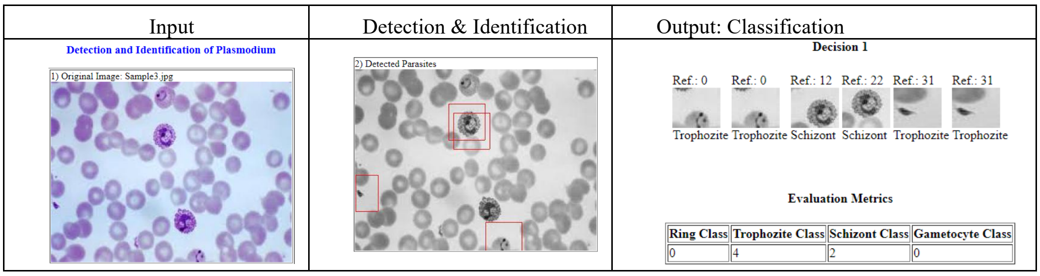
The data were collected from the Division of Parasitic Diseases and Malaria (DPDM) of the Centers of Disease Control and Prevention (CDC). There were two modes of acquisition namely: downloaded directly via the CDC website and in a zip format via email sent by CDC. It is constituted of 40 blood image samples that are anonymous and under agreement of use.

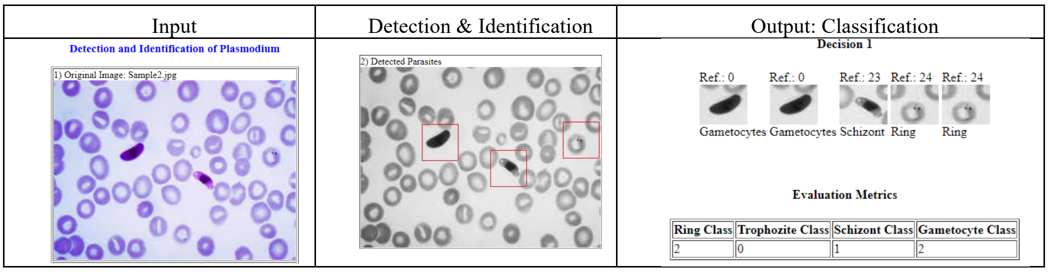
3.1.2 Pre-analytic Phase: Data Characteristics

In laboratory image analysis, geometrical models of particle play an important role in the diagnosis of diseases. Theoretically, we can distinguish different geometric shapes based on some characteristic of the shapes. The experimentation concerns the specie Plasmodium Falciparum. Geometrically, the different morphologies take by the Plasmodium falciparum can be the following: dots, ring, circle and crescent. These the different morphologies are belonging to all staged of Plasmodium namely: ring, trophozoite, Schizont and gametocyte. Moreover, they are designated as clusters (prototypes).

3.1.3 Analytic Phase: Experimentation of the Model

Based on our formal model, we implemented our machine learning algorithms. We present in the figures below the execution of our machine learning and the results of the tests carried out on two images (https://www.vchf.net/vchf/simula/vlab/simulaBrowser.php).





3.1.4 Evaluation Metrics

The table below shows the indicators of performance and demonstrates the learnability of the machine learning algorithms. The accuracy in our unsupervised machine learning means detection and correct classification of all necessary objects in a single image.

Table 1: Indicators of Performance

Image Quantity	40 jpeg images (2D)		
Preparation technique	Giemsa-stained thick blood sample		
Quality	Some images have been affected by chemical added substances or others impurities		
Objects to find	Ring, trophozoite, schizont, gametocyte		
Processing time	<1 min by image		
Results	*Accuracy*	*Specificity and sensitivity (Confusions)*	*Inaccuracy*
	30%	***67,5%***	***2,5%***

4 Discussion

Within the scope of our study, we have formalized and implemented an unsupervised machine learning. The use of machine learning is often justified by the complexity of the problem such as that of decision support and in particular the analysis of images for a diagnosis.

Asking the machine to make a suitable grouping of the objects of an image in classes without human intervention by algorithms, this is the goal of unsupervised machine learning. To achieve this challenge, metrics play an important role.

The formal model presented is based on a set of rules and functions that analyse and classify objects' image in classes.

The model was tested on 40 different images of thick film samples. All these images present different objects with different configurations. The evaluation on these 40 images gives an accuracy of 30%, 67.5% with a difference in precision (mixture of true positives and negative confusions) and 2.5% completely inaccurate. We have considered that the accuracy of unsupervised machine learning is ability to detect and classify correctly of all necessary objects in a single image.

In view of these results, one might be tempted to say that it is always very complex to carry out an unsupervised machine learning. However, it is rather a question of model and therefore of the metrics used that must be refined. It is ultimately important to have knowledge of the mathematical properties of a metric to determine its relevance for a given task.

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It is often difficult to evaluate the performance of a model in unsupervised learning, since the true labels are not known. Furthermore, there are extrinsic factors to the model, namely the quality of the image, which often depends on the acquisition chain.

Taking into account these factors, our model borrowed the principles mentioned in [22] [23], on the Probably Approximately Correct (PAC) Learnability and constructive function approximation.

And if we already validate our model, it may well be useful for semi-supervised machine learning co-clustering applications. This can make it easier to label a large volume of data.

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