

Partial Classification Forest

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Abstract

This paper is concerned with a method I call Partial Classification. It is based on the premise that for a given classification problem a solution must fulfill a certain quality criteria which is not achievable by non-partial classification approaches. For some of these classification problems a partial solution achieving the quality criteria is still useful. A partial solution is a classifier that either predicts an observation or returns nothing if it is not sure enough about the corresponding label.

This paper proposes such a partial classifier, a Monte Carlo based ensemble method called Partial Classification Forest (PCF). The PCF is a Meta Classifier generating instances of a k-d tree like structure in order to partition the feature space of a given dataset. This paper describes the structures and operations of the PCF before showing its application and comparing it to other non-partial classifiers.

Afterwards further features and optimizations of the PCF are discussed. At least conclusions and a roadmap concerning the PCF are presented.

Index Terms—Supervised Machine Learning, Partial Classification, Monte Carlo Method, Meta Classifier

I. Introduction

Some datasets do not allow a classifier to generate a descision surface good enough to be able to predict unseen observations well. A dataset contains tuples of observations and their labels. An observation is a point inside the feature space whereas the label is an element from a finite set called label set. A classification problem is the goal to find a function that maps

the feature space to the label space based on the observations and their respective labels provided by the dataset.[6, chapter 18] This function is called a classifier.

Sometimes a classifier needs to fulfill a certain quality criteria in order to consider it a solution to the respective classification problem. For example think of any classification problem that needs a classifier to have an accuracy of 99 percent, which is impossible to find for a given dataset.

For some of those classification problems it may still be valuable to predict only on partitions of the feature space if the problem is partially solvable. A problem is partially solvable if a classifier should return the label of an observation as the desired output, but can also return nothing if the classifier is “not shure” enough whether it even can return the correct label.

I call this whole concept Partial Classification.

For the example above: if there exists at least one partiton of the feature space in which a classifier can be found that has an accuracy of 99 percent the problem still can be partially solved if this is desired.

More generally accuracy would be the quality metric, the classifier’s accuracy is the quality measurement and 99 percent the quality threshold which must be met by a classifier’s quality measurement in order to consider the classifier a (partial) solution to the classification problem. Any metric, for example a loss metric, can be used to determine a classifier’s quality.

This paper proposes a Monte Carlo based ensemble method called Partial Classification Forest (PCF), which builds an ensemble of trees

having a structure similar to k-d trees to partition the feature space of a given dataset in order to find partitions making Partial Classification possible.

It should be noted here, that this paper is rather a Proof of Concept describing the structures and algorithms of a very early version of the PCF. It has several shortcomings in research and empirical tests, due to a lack of time and no complete, fast implementation. I will discuss these shortcomings further in Chapter VI:

- Tests with a more sofisticated γ (cmp. Section II-A)
- The PCF's performance on high dimensional data
- Untested possible optimizations and features (cmp. Section V)
- A Tree's growing behaviour
- Benchmarks

In Section II I will lay out the structure and the operations of the k-d tree like structure the PCF uses.

In the following text such a tree generated by the PCF is spelled Tree with a capital T, rather than tree, which is used to denote the tree data structure.

In Section III I will describe how the PCF works and utilizes Tree instances. After that I will continue displaying the application of the PCF and compare it to other, non-partial classifiers.

Because this paper is concerned with an early version of the PCF it will also contain a discussion about possible additional features in Section V.

After that I will finish with my conclusions.

II. The Tree structure

A Tree generated by the PCF is a binary search tree structure similar to k-d trees. Its purpose is to randomly generate disjoint partitions of a feature space.

A Tree has two types of nodes, non-leaf nodes, here denoted as Nodes and leaf nodes denoted as Leaves. It provides two operations:

(i) FIT, initializing the Tree and (ii) PREDICT, returning a label for an oberservation.

The Node structure contains three properties: (i) a split value; (ii) a left and (iii) a right successor, both references to either another Node or a Leaf.

A Leaf on the other hand, is the structure representing a partition of the feature space, having the following properties: (i) *active*: a boolean value deciding whether the partition's quality, determined during the FIT operation, is equal or better than the defined threshold or not; (ii) optionally a classifier which is used to classify oberservations during the PREDICT operation. Only if a Leaf's *active* property is true, a classifier must be provided. A Leaf also has two vectors with arbitrary length as properties: (iii) a vector containing the observations of the dataset used in FIT, which are laying inside the partition and (iv) their inherent labels.

During the FIT operation a Tree contains a third type of node, Nil. Nil is used to initialize Trees and the left and right successor of a Node. These nodes are transformed during FIT to either a Node or a Leaf, so after the FIT operation a Tree does not contain Nil nodes anymore. A Nil node does not have any properties.

A. The FIT operation

The FIT operation constructs a Tree, based on a dataset split in observations (X) and their labels (y). Algorithm 1 shows how FIT recursively builds a Tree, which is at the beginning a pointer to a Nil node.

The most important parameter passed to FIT is γ . γ is a function returning (i) a classifier and (ii) the loss of it. Otherwise γ is treated as a black box by the PCF, so what the classifier is and how its loss is calculated are not relevant to the PCF, as long as the classifier is callable¹ and returns an element from the label set when being called (Algorithm 2, line 9). The loss returned by γ gets compared to the quality

¹There could be another interface for the classifier, for example a predict method similar to the scikit-learn library.[\[2\]](#)

threshold τ_l . Is the loss $\leq \tau_l$ the classifier is good enough and Θ is transformed to an active Leaf (Algorithm 1, lines 2, 3).

There are two other thresholds besides τ_l , $\tau_{|X|}$, τ_h . Both regulate the behaviour of a Tree's growth. $\tau_{|X|}$ defines a minimum amount of observations a Leaf must contain. One can easily imagine, without $\tau_{|X|}$ or $\tau_{|X|} = 0$ a Tree would never stop growing, since FIT would continue to split empty partitions, trying to find a smaller partition which would be predictable, even though no classifier could be generated without observations to train it on.

τ_h further regulates the maximum path length of a Tree. It is necessary besides $\tau_{|X|}$, because of the following scenario: be $\tau_{|X|} = 2$ and there are two equal observations in the dataset, but both having a different label than the other one. Now γ , passed X containing only those two identical observations, returns a classifier with a loss $> \tau_l$. Since $|X|$ is still not smaller than $\tau_{|X|}$ FIT would continue trying to separate the two inseparable observations. To prevent such a scenario τ_h tells FIT to stop before the Tree's height, the amount of edges of the longest path, would exceed τ_h . The path length of the Tree's root to Θ is passed as a parameter h to FIT.

Now, if neither τ_l is exceeded nor $\tau_{|X|}$ or τ_h is violated, FIT performs a split and transforms Θ to a Node (Algorithm 1, lines 7ff). The dimension the split is performed on is chosen in a cyclic manner, a practise also applied to k-d trees (Algorithm 1, line 7). [1] But rather than choosing the splitting value at the median of the observations in the dimension, which is done in order to construct balanced k-d trees, the splitting value is random.[1]

In order to chose a proper splitting value β_X is passed as another parameter to FIT. β_X represents the boundaries for every dimension of the feature space based on X . For each dimension β_X contains a tuple with the minimum and maximum value in the dimension of all observations in X .

$\beta_X[\text{dimension}]$ is passed to a pseudo-

random number generator² generating a random value so that $\text{lower}(\beta_X[\text{dimension}]) \leq \text{random number} \leq \text{upper}(\beta_X[\text{dimension}])$ (Algorithm 1, line 8).

Afterwards X , y , β_X are splitted into two new disjoint partitions and FIT is recursively applied to the two new partitions (Algorithm 1, lines 10ff).

Since τ_h is defined, the maximum amount of nodes a Tree can have is $2^{\tau_h+1} - 1$ if the Tree would be perfectly balanced. [7, chapter 16.1] For each node FIT is called, so building a Tree has a worst case time complexity of $\mathcal{O}((2^{\tau_h+1} - 1) * \mathcal{O}(\text{FIT}))$. $\mathcal{O}(\text{FIT})$ is determined by the size of X , since X has to be splitted and by $\mathcal{O}(\gamma)$. That said, a single FIT operation would have a worst case time complexity of $\mathcal{O}(|X| + \mathcal{O}(\gamma))$, which would mean the time complexity of the whole fitting process would be $\mathcal{O}((2^{\tau_h+1} - 1) * (|X| + \mathcal{O}(\gamma)))$.

B. The PREDICT operation

The PREDICT operation traverses a Tree until it encounters a Leaf. If the Leaf is active a label to a provided observation x is returned by the classifier property of the Leaf, otherwise Λ is returned (Algorithm 2).

Λ must not be an element of the label set.

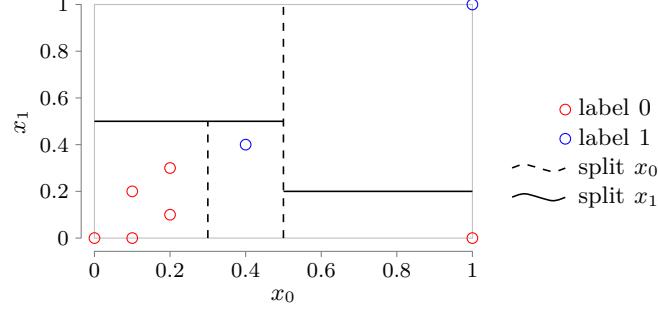
Since the PCF does not predict on its own but instead uses other classifier instances for the actual prediction the PCF is a Meta Classifier.[4, chapter 4.6]

PREDICT is fairly similar to the search operation of a binary tree, except for the type distinction and the prediction.[3, chapter 12.2] Therefore, PREDICT has a worst case time complexity of $\mathcal{O}(\tau_h + \mathcal{O}(\text{classifier}))$.

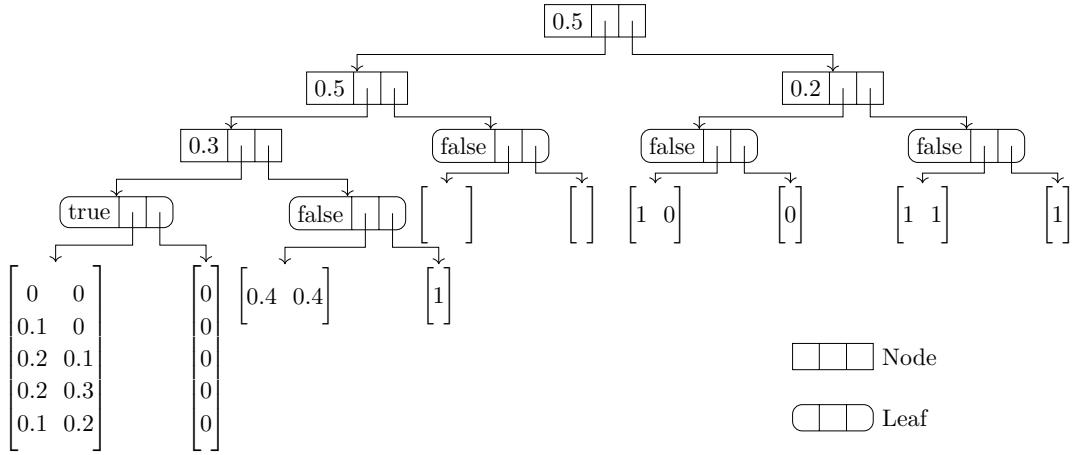
III. Partial Classification Forest

The PCF has two parameters, (i) N and (ii) an array with N pointers. N is the amount of Trees the PCF maintains. Initially the pointers inside the array are references to Nil nodes.

²The implementation uses Python 3.6's random library.[8, chapter 9.6]



(a) Scatterplot showing the observations and the splits done by the FIT operation.



(b) The structure of the Tree generated by FIT.

Fig. 1: Example of FIT on a dataset seen in Figure 1a. γ simply computes the probability of each label in y and returns a function returning the label with the maximum probability and as loss 1 - the maximum probability. The thresholds are: $\tau_l = 1$, $\tau_{|X|} = 2$. τ_h can be any integer above 2.

The PCF offers the same two operations a Tree has, FIT (Algorithm 3) and PREDICT (Algorithm 4), both abstractions to the equivalent Tree operations.

Once FIT is executed, the pointers are references to the roots of fitted Tree instances.

Both FIT and PREDICT can be implemented as multithreaded operations as long as γ is threadsafe, since the Tree instances are independent of each other and the shared parameters X , y (FIT) and x (PREDICT) are read only, making synchronization unnecessary.

FIT first computes β_X which has a time complexity of $\mathcal{O}(|X[0]| * |X|)$, $|X[0]|$ denoting the amount of dimensions the feature space has.

After that the Tree's FIT operation is called N times, which means the PCF's FIT operation has a worst case time complexity of $\mathcal{O}(N * (2^{\tau_h+1} - 1) * (|X| + \mathcal{O}(\gamma)) + |X[0]| * |X|)$ (cmp. Section II-A).

The PCF's PREDICT operation first initializes an array with N elements (Algorithm 4, line 1). Each Tree instance fills one element of the array with its prediction. After that the PCF's

Algorithm 1 : FIT($\Theta, X, y, h, \beta_X, \gamma, \tau_l, \tau_{|X|}, \tau_h$)

A Tree's FIT operation.

Inputs:

- Θ – a pointer to a Nil node; initially pointing to the root node of an empty Tree,
- X – input data,
- y – labels of X ,
- h – height of the Tree; initially $h = 0$,
- β_X – lower and upper boundries of every dimension of X ,
- γ – function returning a classifier and its loss,
- τ_l – loss threshold,
- $\tau_{|X|}$ – threshold for the size of X ,
- τ_h – height limit of the Tree

Output: void

- 1: classifier, loss $\leftarrow \gamma(X, y)$
 - 2: if loss $\leq \tau_l$ then
 - 3: $\Theta \leftarrow \text{LEAF}(\text{true}, \text{classifier}, X, y)$
 - 4: else if $h > \tau_h$ or $|X| < \tau_{|X|}$ or loss $> \tau_l$ then
 - 5: $\Theta \leftarrow \text{LEAF}(\text{false}, \text{classifier}, X, y)$
 - 6: else
 - 7: dimension $\leftarrow h \bmod |X[0]|$
 - 8: split $\leftarrow \text{RANDOM}(\beta_X[\text{dimension}])$
 - 9: $\Theta \leftarrow \text{NODE}(\text{split}, \text{NIL}, \text{NIL})$
 - 10: split X, y and β_X into $X', X'', y', y'', \beta'_X, \beta''_X$
 - 11: FIT($\Theta.\text{left}, X', y', h + 1, \beta'_X, \dots$)
 - 12: FIT($\Theta.\text{right}, X'', y'', h + 1, \beta''_X, \dots$)
 - 13: end if
-

PREDICT operation takes the label predicted most and returns it as its prediction for the observation x (Algorithm 4, lines 5, 6).

The worst case time complexity of the PCF's PREDICT operation is $\mathcal{O}(N * (\tau_h + \mathcal{O}(\text{classifier})) + N)$, since a Tree's PREDICT operation is executed N times, plus the most predicted label must be determined, which is $\mathcal{O}(N)$.

IV. Application

This Section will further outline the use case of the PCF, display results of a test on an artif-

Algorithm 2 : PREDICT(Θ, x, h)

A Tree's PREDICT operation.

Inputs:

- Θ – a Tree node; initially pointing to the root of the Tree,
- x – an observation,
- h – height of the Tree; initially $h = 0$

Output: the predicted label or Λ

- 1: if TYPE(Θ) is Node then
 - 2: dimension $\leftarrow h \bmod |x|$
 - 3: if $x[\text{dimension}] \leq \Theta.\text{split}$ then
 - 4: PREDICT($\Theta.\text{left}, x, h + 1$)
 - 5: else
 - 6: PREDICT($\Theta.\text{right}, x, h + 1$)
 - 7: end if
 - 8: else if $\Theta.\text{active}$ then
 - 9: return $\Theta.\text{classifier}(x)$
 - 10: else
 - 11: return Λ
 - 12: end if
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Algorithm 3 : FIT($\Pi, X, y, \gamma, \tau_l, \tau_{|X|}, \tau_h$)

The PCF's FIT operation.

Inputs:

- Π – a PCF instance,
- X – input data,
- y – labels of X ,
- γ – function returning a classifier and its loss,
- τ_l – loss threshold,
- $\tau_{|X|}$ – threshold for the size of X ,
- τ_h – height limit of the Tree

Output: void

- 1: compute β_X
 - 2: for all $\Theta \in \Pi.\text{trees}$ do
 - 3: FIT($\Theta, X, y, 0, \beta_X, \dots$)
 - 4: end for
-

Algorithm 4 : PREDICT(Π, x)

The PCF's PREDICT operation.

Inputs:

Π – a PCF instance,

x – an observation,

Output: the predicted label or Λ

```

1: predictions  $\leftarrow [\Lambda; N]$ 
2: for  $i = 1$  to  $N$  do
3:   predictions[ $i$ ] = PREDICT( $\Pi.\text{trees}[i], x, 0$ )
4: end for
5: determine  $l_{max}$ , the label predicted most
6: return  $l_{max}$ 

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ical dataset and compare it to other classifiers. Furthermore a test of the PCF's behaviour with different amounts of Trees will be shown.

Both tests are performed on a randomly generated, normalized, two dimensional and binary labeled dataset. The dataset contains five thousand observations and was designed to be unpredictable, when predicted as a whole. The plane from which the observations are generated contains five partitions in which the observations all have the same label. Observations from those five partitions make up twenty percent of all observations and are the only ones which should be predicted, because all points not inside those partitions are labeled randomly. The optimal descision surface would be equal to the area of the five partitions.

All observations are generated by a pseudo-random number generator[8, chapter 9.6], therefore, every point on the plane has the same probability to be chosen as an observation for the dataset.

The dataset is designed this way in order to be able to show the application of the PCF in the domain of partial classification. Only twenty percent of the whole dataset is predictable which makes it impossible for other, non-partial classifiers to be able to find an adequate descision surface. The following tests all take $\tau_l = 1$ as quality threshold which is impossible to achieve

predicting on the whole dataset.

It is common practise in machine learning to split a dataset into a training and a test set in order to find the best model.[6, chapter 18] This approach is also used for the PCF. The training set is used as the parameters X and y of FIT (Algorithm 3) while PREDICT (Algorithm 4) is used on every observation of the test set.

Two metrics are used to describe the behaviour of the PCF, (i) *predicted* and (ii) *accuracy*. Both metrics are derived from comparing the label of an observation returned by PREDICT with its actual label from the dataset.

Predicted is the percentage of predicted observations, while *accuracy* is the percentage of correctly classified observartions from the test set. *Accuracy* is used as the quality measurement, which means in the context of this tests, every classifier not able to achieve *accuracy* = 1 is not acceptable.

For both tests γ , τ_l and τ_h are the same. γ and τ_l are equal to the values used in Figure 1 while $\tau_h = 32$. The dataset was splitted into a training and a test set such that ten percent of the observations were used as the test set.³ The observations were chosen randomly.

The first test will show the descision surface of the PCF with different N and $\tau_{|X|}$. For the test three different values, two, five and ten were used for both N and $\tau_{|X|}$ to show how those two parameters change the descision surface of the PCF. The test shows that for $\tau_{|X|} = 2$ the PCF overfitted the data, which means that *predicted* exceeded twenty percent, the amount of accurate observations while also failing to meet an *accuracy* equal to τ_l . This results in the chaotic descision surfaces shown in Figures 2a - 2c. On the other hand for $\tau_{|X|} = 10$ the descision surface is very small which means the PCF's *predicted* is far less than twenty percent (Figures 2g - 2i).

How non-partial classifiers perform on the dataset can be seen in Figure 3. Three common

³For splitting scikit-learn's `model_selection.train_test_split` was used during the tests.[2]

classifiers are tested, all from the scikit-learn library.[2] Their parameters are the standard parameters given by scikit-learn. Tested were the Support Vector Machine, Random Forest and K Nearest Neighbors, where K in this case is five.[2] Figure 3 also shows the *accuracy* of these classifiers. None are close to $\tau_l = 1$.

The second test shows the influence the amount of Trees N has on *predicted* and *accuracy*. In this test $\tau_{|X|}$ equals four.

Figure 4 shows that, for this dataset with the chosen thresholds, the PCF instances with $N < 30$ variate, both their *predicted* and *accuracy* values. Is $30 \leq N \leq 100$ *accuracy* is constant and equals τ_l . *Predicted* on the other hand, still rises in this interval. Is $N \geq 100$ *predicted* is higher than *predicted* with $N = 100$ and constant, but *accuracy* fails to meet τ_l , which means the PCF instances are overfitting.

Furthermore the second test relates *predicted* and *accuracy* of the observations from the test set to the values for the training set, showing that more training observations are predictable than test observations (cmp. Figure 4).

V. Possible additional features

There are some possible features and optimizations to the PCF which were not discussed in the previous Sections. Again it should be noted that these features and optimizations are yet untested (see Introduction).

The proposed features are:

- 1) Weighing partitions.
- 2) Densifying a Tree after FIT.
- 3) Chosing the dimension a Node has randomly rather than cyclic (cmp. Section II-A).
- 4) Add a rotation matrix to every Tree.
- 5) A second, more light-weight variant of the PCF reducing the memory usage, depending on γ .

The first feature would be to weigh partitions. As of right now, the PCF's PREDICT operation determines l_{max} as the label predicted most (Algorithm 4, line 5).

This could be further refined with weighing each partition based on two properties: (i) the amount of observations a partition contains and (ii) its volume. This would result in a weight determined as:

$$\text{weight} = \frac{|\text{partition}.X|}{V(\text{partition})}. \quad (1)$$

A partition with a lot of observations and a small volume would have a higher weight than one with a small amount of observations and a high volume, further increasing the probability that the label predicted by the partition with the higher weight is determined as l_{max} . So instead of just counting each label predicted and returning the one predicted most, the weight of each prediction is summed and the label with the highest sum will be returned by PREDICT as l_{max} .

The second optimization is densifying a Tree after FIT. If a Node has two inactive Leaves as children the Node is unnecessary since either way Λ is returned. The Node could be transformed into an unactive Leaf, reducing the path length of the branch by one and decreasing the amount of nodes by two, which decreases the size of the Tree and therefore the time complexity of PREDICT.

Two features inspired by methods used in the Approximate Nearest Neighbor Search are (i) chosing the splitting dimension, like the splitting value, at random rather than cyclic (cmp. Section II-A) and (ii) also rotating the data for each Tree instance.[5, pages 17 - 27] This further increases the possibility of having Trees with different structures and therefore partitions.[5, page 24]

In Section IV and in Figure 1 a very simple classifier is returned by γ . It only computes the probability for each label and returns the label with the highest probability (cmp. Figure 1).

A classifier like that does not need to know where the observations are in the partition which makes it unnecessary to keep them in a Leaf node as X and y (cmp. Algorithm 1). Instead a dictionary with every label from the label space where each label is mapped to the amount

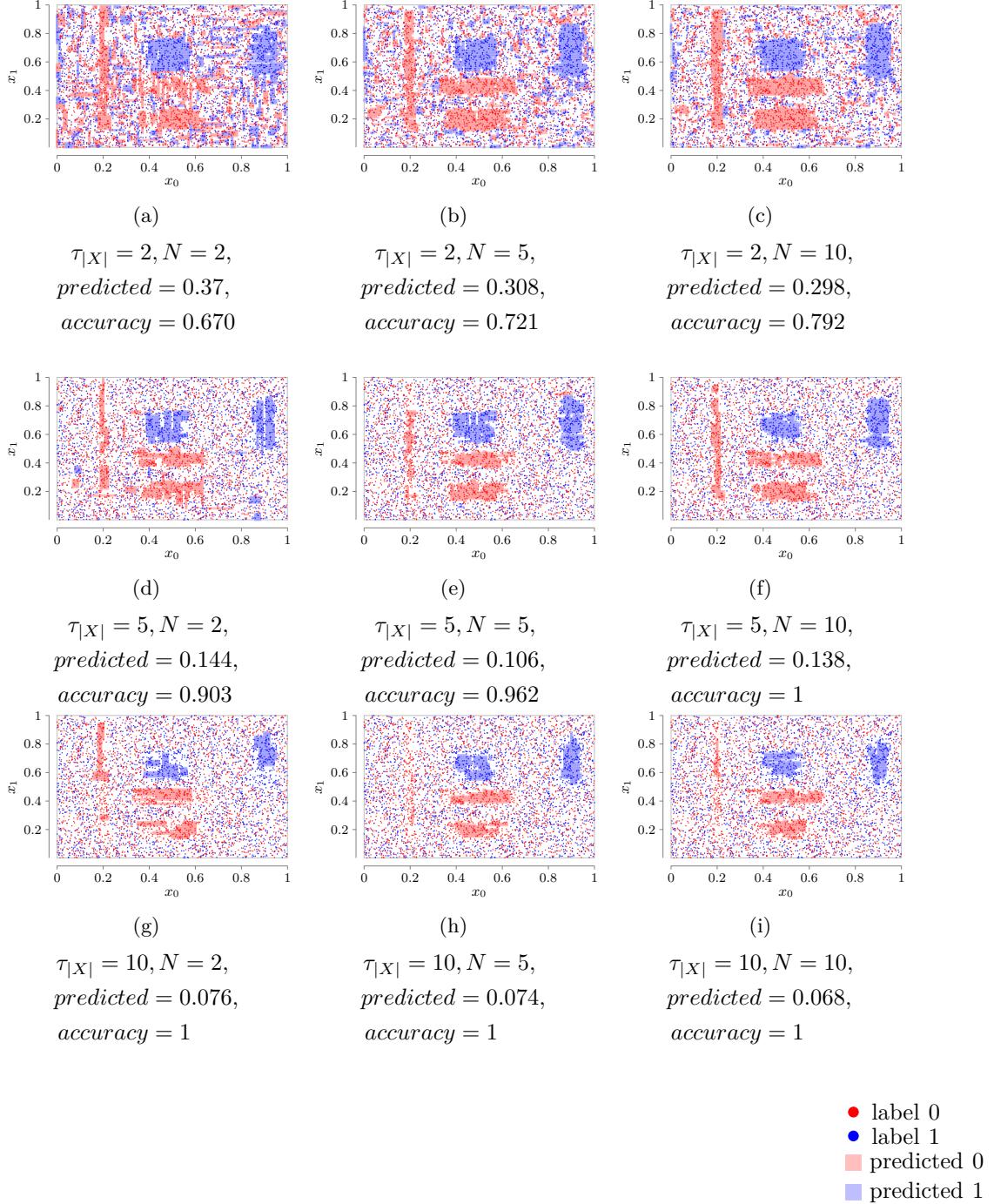


Fig. 2: The descision surfaces of differently configured PCFs. The threshold $\tau_{|X|}$ and the amount of Trees N of the PCF are different for each Figure, 2a - 2i.

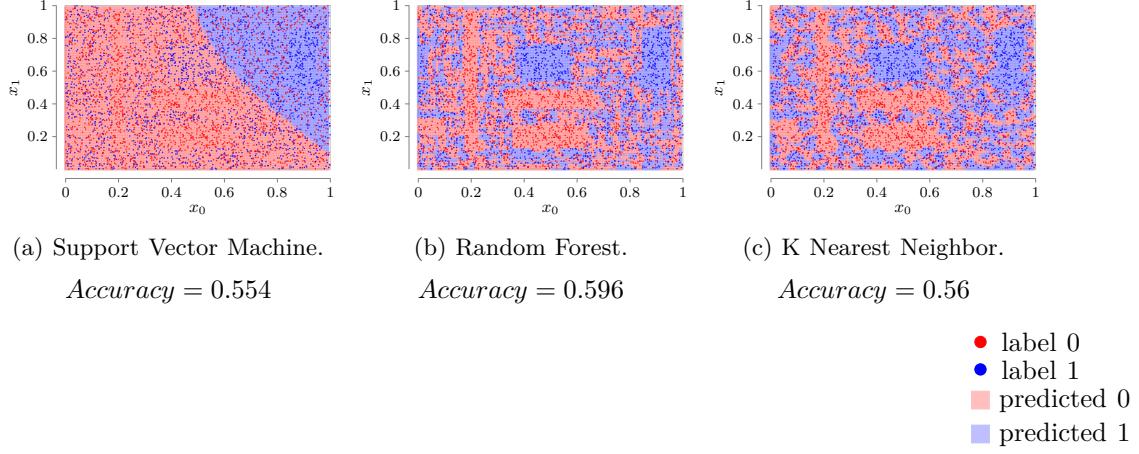


Fig. 3: The descision surfaces of other classifiers than the PCF.

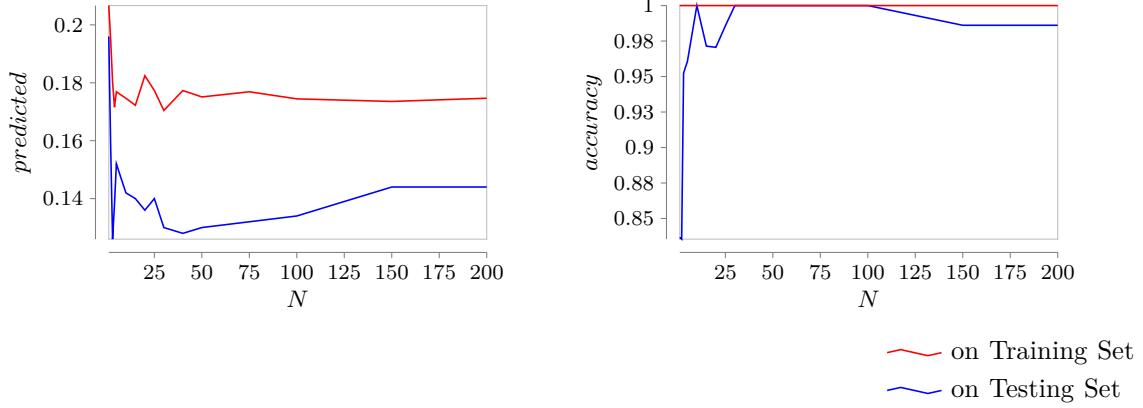


Fig. 4: The amount of Trees of the PCF N , in relation to *predicted* and *accuracy*.

of observations inside the partition having the particular label is enough.

A possible feature would be to provide a second variant of the PCF which passes this dictionary instead of the observations to γ , decreasing the complexity of the PCF for classifiers which do not need to know where each observations lays inside the partition.

VI. Conclusions

In the Introduction I described what I mean by Partial Classification. The whole concept is

based on the condition that a classifier needs to maintain a certain quality in its predictions for a given classification problem. If it can not do this, it is not regarded a solution.

Partial Classification is a way to still find classifiers that partially solve a classification problem not solvable as a whole. A partial classifier only predicts the label of an observation if it lays inside a partition it can classify. Otherwise it returns nothing, indicating that the classifier is not sure which label the observation has.

This paper provides a description of such

a partial classifier, the Partial Classification Forest. It describes the core structures and operations of the PCF and shows its use on an artificial problem designed to display the use of it over other, non-partial classifiers.

Also stated in the Introduction, this paper has some shortcomings in research and empirical tests regarding the PCF, due to a lack of time and no complete, fast implementation. A list of these shortcomings is also provided in the Introduction. The next step will be to make a fast and complete implementation before proceeding with the research and the empirical tests.

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