Abstract. The k nearest neighbor \((k\text{-NN})\) classifier has been extensively used in Pattern Recognition because of its simplicity and its good performance. However, in large datasets applications, the exhaustive \(k\text{-NN}\) classifier becomes impractical. Therefore, many fast \(k\text{-NN}\) classifiers have been developed; most of them rely on metric properties (usually the triangle inequality) to reduce the number of prototype comparisons. Hence, the existing fast \(k\text{-NN}\) classifiers are applicable only when the comparison function is a metric (commonly for numerical data). However, in some sciences such as Medicine, Geology, Sociology, etc., the prototypes are usually described by qualitative and quantitative features (mixed data). In these cases, the comparison function does not necessarily satisfy metric properties. For this reason, it is important to develop fast \(k\) most similar neighbor \((k\text{-MSN})\) classifiers for mixed data, which use non-metric comparison functions. In this thesis, four fast \(k\text{-MSN}\) classifiers, following the most successful approaches, are proposed. The experiments over different datasets show that the proposed classifiers significantly reduce the number of prototype comparisons.

Keywords: Nearest neighbor rule, fast nearest neighbor search, mixed data, non-metric comparison functions.

1 Introducción

The \(k\text{-NN}\) classifier (Cover & Hart, 1967) has been widely used in Pattern Recognition, because of its simplicity and its good performance. The \(k\text{-NN}\) classifier uses a training set \((T)\) of prototypes, whose class is known \(a\ priori\). To decide the class of a new prototype, the \(k\text{-NN}\) classifier performs an exhaustive comparison between the prototype to classify and the prototypes in the training set, assigning to the new prototype a class, according to the classes of its \(k\) nearest neighbors in \(T\). However, when the training set is large, the exhaustive
comparison is expensive and sometimes inapplicable. Thus, many fast k-NN classifiers have been designed; different reviews appear in (Nene & Nayar, 1997; Ramasubramanian et al., 2000; and Yong-Sheng et al., 2007).

The objective of a fast k-NN classifier is to reduce the number of comparisons trying to keep the classification accuracy obtained by k-NN. Speeding up the k-NN classifier is required because some applications demand a rapid response on large datasets, for example online stock analysis, air traffic control, network traffic management, intrusion detection, etc. Also, fast k-NN classifiers are useful for problems with high dimensionality where the comparison function could be very expensive (Mico et al., 1994; Denny & Franklin, 2006), under this context, reducing the number of comparisons could be very important. For these reasons, although nowadays the computers are very fast, the development of fast k-NN classifiers is currently an active research area (Adler & Heeringa, 2008; Panigrahi, 2008). Nevertheless, most of the fast k-NN classifiers proposed in the literature have been designed for numerical prototype descriptions compared through a metric function. Moreover, in some sciences such as Medicine, Geology, Sociology, etc., the prototypes are usually described by numerical and non numerical features (mixed data) and the comparison function does not satisfy metric properties.

Thus, if a metric is not available but a comparison function that evaluates the similarity between a pair of prototypes can be defined, given a new prototype Q to classify, the objective is to find the k most similar neighbors to Q in a training set T (with N prototypes, where each prototype is described by d attributes, which can be numerical or non numerical), and assign to Q a class (based on its k most similar neighbours). However, the exhaustive search of the k-MSN, as occurs with k-NN, could be very expensive if T is large. For this reason, it is important to develop fast k most similar neighbor (k-MSN) classifiers for mixed data and non metric comparisons functions.

In this thesis, four fast k-MSN classifiers are proposed. The first uses a tree structure, the second and the third are based on a new Approximating-Eliminating approach for mixed data. Finally, the last fast k-MSN classifier proposed in this thesis uses a tree structure and an Approximating-Eliminating approach. In order to evaluate the proposed fast k-MSN classifiers, some experiments over real datasets were performed, comparing against other fast k-NN classifiers. From these experimental comparisons, we could notice that using the proposed methods competitive classification accuracy was obtained, but with less prototype comparisons.

This work is organized as follows: Section 2 provides a brief review of fast k-NN classifiers. In Section 3-6, our fast k-MSN classifiers (Tree k-MSN, AEMD, LAEMD, Tree LAEMD) are introduced. In Section 7, experimental results, obtained using our classifiers and a comparison against other fast classifiers, are reported. Finally, in Section 8 we present our conclusions and future work.

2 Related work

In order to apply the k-NN classifier to problems where the training set is large, in the last years, several fast k-NN classifiers have been proposed. The objective of a fast k-NN classifier is to reduce the number of comparisons trying to keep the classification accuracy obtained by k-NN.

The fast k-NN classifiers can be divided in exact and approximated methods. Using exact fast k-NN classifiers, the same classification accuracy as using the exhaustive k-NN classifier are obtained. Approximated methods do not guarantee to find the k nearest neighbors from the training set, but they find an approximation faster than the exact methods.

According to the strategy used to avoid prototype comparisons, fast k-NN classifiers can be divided as shown in table 1. From this table, we can observe that most of the existing fast k-NN classifiers are proposed to work with numerical data and metric comparison functions. For this reason, in this thesis four fast k most similar neighbor (k-MSN) classifiers for mixed data and non metric comparisons functions are proposed. To develop these methods, the most successful approaches from the state of the art (Partitioning, Approximating-Eliminating and Hybrid methods) where followed. The proposed methods are described in the next sections.
Table 1. Fast k-NN classifiers divided according to the strategy used to avoid prototype comparisons; X means that there was not any work in that category.

<table>
<thead>
<tr>
<th>FAST k-NN CLASSIFIERS</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>1. For metric functions</strong></td>
</tr>
<tr>
<td><strong>Exact methods</strong></td>
</tr>
<tr>
<td><strong>I. Partial distance search</strong></td>
</tr>
<tr>
<td>(Cheng 1984)</td>
</tr>
<tr>
<td>(Hwang 1998)</td>
</tr>
<tr>
<td><strong>II. Projection methods</strong></td>
</tr>
<tr>
<td>(Friedman, 1977)</td>
</tr>
<tr>
<td>(Funck, 1976)</td>
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<tr>
<td>(Nene and Nayar, 1997)</td>
</tr>
<tr>
<td><strong>III. Approximating-Eliminating</strong></td>
</tr>
<tr>
<td>AESA (Vidal, 1986), LAESA (Mico et al., 1994)</td>
</tr>
<tr>
<td>iAESA probabilístico (Figueroa et al., 2006)</td>
</tr>
<tr>
<td><strong>IV. Partitioning and Tree-based methods</strong></td>
</tr>
<tr>
<td>Kd-tree (Friedman et al., 1975)</td>
</tr>
<tr>
<td>R-tree (Guttman, 1984)</td>
</tr>
<tr>
<td>Modificaciones de R-tree:</td>
</tr>
<tr>
<td>R*-tree (Breckmann, 1990)</td>
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<tr>
<td>SS-tree (White &amp; Jain, 1996)</td>
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<tr>
<td>SR-tree (Katayama &amp; Satoh, 1997)</td>
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<td>Udler &amp; Heeringa, 2008)</td>
</tr>
<tr>
<td>FN (Fukunaga, 1976)</td>
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<tr>
<td>Modificaciones de FN:</td>
</tr>
<tr>
<td>(Kalantari, 1983)</td>
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<tr>
<td>(Omachi, 2000)</td>
</tr>
<tr>
<td>iGomez-Ballester et al., 2006)</td>
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<tr>
<td>(Oncina et al., 2007)</td>
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<tr>
<td>Metric trees (Uhlmann, 1991)</td>
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<td>Vp-Trees (Yianilos, 1993)</td>
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<td>PAT (McNames, 2001)</td>
</tr>
<tr>
<td>LBT (Yong-Sheng et al., 2006)</td>
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<tr>
<td>List of Clusters (LC) (Chavez &amp; Navarro, 2005)</td>
</tr>
<tr>
<td>Hierarchy of Clusters (Fredriksson, 2007)</td>
</tr>
<tr>
<td><strong>V. Hybrid methods (using Partitioning and Approximating-Eliminating)</strong></td>
</tr>
<tr>
<td>TLAESA (Mico et al., 1996)</td>
</tr>
<tr>
<td>Modificación de TLAESA (Tokoro, 2006)</td>
</tr>
<tr>
<td><strong>2. For non metric functions</strong></td>
</tr>
<tr>
<td><strong>I. Partitioning and Tree-based methods</strong></td>
</tr>
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<td></td>
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<tr>
<td>DynDe (Goh, et al., 2002)</td>
</tr>
<tr>
<td>Cluster based tree (Zhang &amp; Srivari, 2004)</td>
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</tbody>
</table>

3 Tree k-MSN

The first proposed classifier, Tree k-MSN (Hernández-Rodríguez-a et al., 2007; Hernández-Rodríguez-b et al., 2007), consists of two phases. The first one, or preprocessing phase, builds a tree structure from the training set (T). In the second phase, two search algorithms, which are independent of metric properties of the comparison function, are proposed for classifying a new prototype.

3.1 Preprocessing phase of Tree k-MSN

In this phase, the training set is hierarchically decomposed to create a tree structure (TS). At the beginning, the root of the tree contains the whole training set. In order to create the following levels of the tree, each node n of the tree is divided in C clusters, in such a way that each cluster represents a descendant node of n. Each descendant node is divided again and this process is repeated until a stop criterion is satisfied.
Since our algorithm is designed to allow mixed data, instead of using the C-Means algorithm for building the tree structure, as in the FN classifier, the C-Means with Similarity Functions algorithm (CMSF) (García-Serrano & Martínez-Trinidad, 1999), is used. CMSF allows creating C clusters and computing as representative element of each cluster a prototype belonging to the cluster (i.e., a prototype contained in T); besides CMSF allows using any similarity function.

Each node p of the tree contains three features: S_p the set of prototypes that belong to p; N_p the number of prototypes in p and unlike FN and MS classifiers, Rep_p a representative prototype of the node, which is on average the most similar to the rest of prototypes in the node.

A node is marked as a leaf when a stop criterion is satisfied. In this thesis we used a stop criterion based on the node size (SC1), which is used in (Fukunaga & Narendra, 1975; Kalantari & McDonald, 1983; Mico et al., 1996; Omachi & Aso, 2000; McNames, 2001; D’Haes et al., 2002; Gomez-Ballester et al., 2006) and we introduce two new stop criteria (SC2 and SC3), which take into account not only the number of prototypes of the node, but also the class distribution of these prototypes. The three stop criteria are the following:

1. Stop criterion 1 (SC1). This criterion is based on the node size. According to this criterion, if the number of prototypes contained in a node is less than a predefined threshold (N_p ≤ NoP), then the node is marked as a leaf. The objective of this criterion is to obtain leaves with a few prototypes. However, when most of the prototypes contained in a node belong to the same class, dividing this node could lead to unnecessary prototype comparisons during the classification stage, between the prototype to classify and the representative prototypes of the nodes. Because all descendant nodes, that would be created, also would belong to the same class. Since the objective is to classify a new prototype trying to avoid prototype comparisons, we propose a second stop criterion during the tree construction:

2. Stop criterion 2 (SC2). If most of the prototypes in a node belong to the same class, then the node is considered as a leaf and it is marked with the majority class, even if the set is not small enough according to the first stop criterion (N_p > NoP). In order to decide how many prototypes in the node must belong to the same class, for generalizing the class of a node, a percentage threshold (PercThres) is used. In the nodes where this criterion is not satisfied, only the size of the node is considered to create leaf nodes (SC1).

When the node is generalized by the majority class, through SC2, if PercThres=100%, it means that all prototypes in the node belong to the same class (the generalized class of the node). However, when PercThres<100%, an error is introduced, because some prototypes in the node do not belong to the majority class. Therefore, we introduce a third criterion:

3. Stop criterion 3 (SC3). If a certain percentage (PercThres) of the prototypes in a node belongs to the same class, two nodes are created. Using the prototypes that belong to the majority class, a leaf node is created and it is marked with the majority class. The rest of the prototypes are assigned to a second node. In the second node, the size is considered to decide if the node is a leaf (if N_p ≥ NoP) or if the node will be divided again. In the nodes where SC3 criterion is not satisfied, only the size of the node is considered to create leaf nodes (SC1).

Using SC2 and SC3 the number of prototype comparisons (during the classification stage) is reduced, because if during the tree traversal a leaf node (marked with the majority class) is reached, then only the representative prototype of the node, with the corresponding majority class, is used to update the list of the k most similar neighbors (only one comparison), instead of comparing the prototype to classify against all the prototypes contained in the leaf.

3.2 Classification phase of Tree k-MSN

In this phase, in order to avoid an exhaustive tree traversal, fast k-NN classifiers rely on pruning rules (based on metric properties). As we are looking for a method applicable when the comparison function does not satisfy metric properties, pruning rules based on the triangular inequality cannot be used; therefore, we propose to stop the search when a leaf of the tree is reached. In the first search algorithm (DF search), we propose to use a depth-first search strategy and in the second search algorithm (BF search), we propose to use a best-first search strategy. The two proposed algorithms for searching the k-MSN are described below:

1. DF search: It begins at the root of the tree, following the path of the most similar node and finishes when a leaf is reached. As each node of the tree is represented by a prototype of the training set, with known class, a list of the k-MSN is stored and updated during the tree
traversal. When the first leaf node \( l \) is reached, if \( l \) is marked with the majority class, then only the representative prototype \( \text{Rep}_l \) is used to update the \( k\)-MSN (because most of the prototypes in the node belong to the same class). If the node is not marked with the majority class, then an exhaustive search in the node is done and the list of \( k\)-MSN is updated. After a leaf is processed, if the list of \( k\)-MSN does not have \( k \) elements, then the tree traversal follows backtracking steps to explore nodes closer to \( Q \), until \( k \) most similar neighbours are found.

2. BF search: It begins at the root of the tree, comparing \( Q \) against the descendant nodes of the root, which are added to a list \( \text{List}_{\text{tree traversal}} \). After that, \( \text{List}_{\text{tree traversal}} \) is sorted in such a way the most similar node to \( Q \) is in the first place. The most similar node (first element) is eliminated from \( \text{List}_{\text{tree traversal}} \) and its descendant nodes are compared against \( Q \), and added to \( \text{List}_{\text{tree traversal}} \), which is sorted again. The search finishes when the first element of \( \text{List}_{\text{tree traversal}} \) is a leaf. In this search, it is possible to reconsider nodes in levels of the tree already traversed if the first node of \( \text{List}_{\text{tree traversal}} \) belongs to a previous level in the tree.

During the tree traversal, another list \( \text{List}_k\)-MSN containing the \( k \) current MSN is stored and updated. After a leaf is processed (in a similar way than in the local search), if \( \text{List}_k\)-MSN does not contain \( k \) elements (MSN), then the first element in \( \text{List}_{\text{tree traversal}} \) is considered to follow a new route. The process stops when \( \text{List}_k\)-MSN contains \( k \) elements (MSN). However, using both search strategies (DF and BF), in practical problems where the training set is large, it is quite difficult that \( \text{List}_k\)-MSN does not have \( k \) elements (MSN) when the first leaf is reached.

After finding \( k\)-MSN, the majority class is assigned to the new sample \( Q \).

In figure 1 the difference between both search algorithms is shown. As we can see, BF search allows evaluating nodes in already traversed levels.

![Figure 1. Example of the search algorithms](image)

### 4 AEMD

The second fast \( k\)-MSN classifier proposed in this thesis, AEMD (Hernandez-Rodriguez-c et al., 2008), is based on a new Approximating-Eliminating approach for Mixed Data. AEMD also consists of two phases: preprocessing and classification, which are described in the next sections.

#### 4.1 Preprocessing phase of AEMD

In this stage, AEMD computes and stores the next information which is used during the classification phase to reduce the number of comparisons between prototypes:

1. **Similarity binary array (SimArray).** In this thesis, we proposed computing and storing an array of similarities per attribute among the prototypes in the training set \( T \), where \( \text{SimArray}(P_a, P_b, x_i) = 1 \) if the prototypes \( P_a \) and \( P_b \) are similar regarding the attribute \( x_i \), \( i \epsilon [1, d] \) and otherwise \( \text{SimArray}(P_a, P_b, x_i) = 0 \), \( P_a, P_b \epsilon T \).

In order to evaluate the similarity per attribute between two prototypes, different approaches can be applied. In this thesis, the following criteria were used:

\[
\text{SimArray}(P_a, P_b, x_i) = C_i(x_i(P_a), x_i(P_b)) \quad (1)
\]

If the attribute \( x_i \) is not numeric:
\[ C_i(x_i(P_a), x_i(P_b)) = \begin{cases} 1 \text{ if } x_i(P_a) = x_i(P_b) \\ 0 \text{ otherwise} \end{cases} \] (2)

If the attribute \( x_i \) is numeric:

\[ C_i(x_i(P_a), x_i(P_b)) = \begin{cases} 1 \text{ if } |x_i(P_a) - x_i(P_b)| < \sigma_i \\ 0 \text{ otherwise} \end{cases} \] (3)

Where \( \sigma_i \) is the standard deviation of the attribute \( x_i \) in \( T \). The required space to store \( SimArray \) is \(|T| \times |T| \times d\), but each element is a bit, therefore \(|T| \times |T| \) words of \( d \) bits are needed for storing \( SimArray \).

2. **Similarity threshold (SimThres)**. This value is used during the tree traversal algorithm to decide if a representative prototype of a node of the tree can be used to prune nodes in the tree. In this thesis \( SimThres \) is computed as follows: let \( Set_c \) be the set of prototypes that belong to class \( c \) (\( c = 1, \ldots, \) number of classes in \( T \)) and \( ClassAvgSim \) be defined as follows:

\[ ClassAvgSim(c) = \frac{\sum_{p_a \in Set_c} \text{ASim}(P_a)}{|Set_c|} \] (4)

\( SimThres \) is computed as the average value of similarity for all the classes:

\[ SimThres = \text{average}(ClassAvgSim(c)) \] (5)

3. **A representative prototype per class (RPc)**. Taking advantage of the class information, we propose to use a representative prototype (RPc) for each class in the training set. These prototypes are used to obtain a first approximation of the \( k \) most similar neighbors during the classification phase, before performing \( TS \) tree traversal algorithm. In this thesis, to compute \( RP_c \), set \( Set_c \) be the set of prototypes that belong to class \( c \). For each \( P_i \) in \( Set_c \):

\[ \text{ASim}(P_i) = \frac{\sum_{j=1}^{\text{|Set_c|}} \text{Sim}(P_i, P_j)}{|Set_c|} \] (6)

Where \( \text{Sim} \) is a similarity comparison function. Thus, the representative prototype for each class is the one that maximizes \( \text{ASim} \) function:

\[ RP_c = \text{argmax}(\text{ASim}(P_i)) \] (7)

Where \( i = 1, \ldots, |Set_c| \), \( c = 1, \ldots, \text{NoClasses} \) and \( \text{NoClasses} \) is the number of classes in \( T \).

### 4.2 Classification phase of AEMD

Given a new prototype \( Q \) to classify, \( SM \), \( RP_c \), and \( SimThres \) (computed during the preprocessing phase) are used to avoid prototype comparisons. The classification phase of AEMD, which is depicted in Figure 2, is based on Approximating-Eliminating steps for mixed data, which are not based on the triangle inequality. This stage is as follows:

- **Initial approximating step.** At the beginning of the algorithm, the prototype \( Q \) is compared against the class representative prototypes per class \( \text{(RP}_c \text{)} \), to obtain a first approximation to the \( k \) most similar neighbors and, in particular, the current most similar neighbor \((\text{Current}_MSN)\). After that, all \( \text{RP}_c \) are eliminated from \( T \).

  - If \( \text{Sim}(Q, \text{Current}_MSN) \geq \text{SimThres} \), then the prototype \( \text{Current}_MSN \) is used to eliminate prototypes from \( T \) (Eliminating step). In other case, the Approximating step is performed.

- **Eliminating step.** In this step, \( \text{Current}_MSN \) is used to eliminate prototypes from \( T \). First, a binary representation \((BR)\) containing the similarity per attribute, between \( Q \) and \( \text{Current}_MSN \) is created as follows:

\[ BR(Q, \text{Current}_MSN) = C_i(X_i(Q), x_i(\text{Current}_MSN)), i = 1, \ldots, d \] (8)

Thus, \( BR(Q, \text{Current}_MSN) = 1 \), if \( Q \) and \( \text{Current}_MSN \) are similar in the attribute \( x_i \) and \( BR(Q, \text{Current}_MSN) = 0 \), in other case. Using \( BR \), those prototypes in \( T \), which are not similar to \( \text{Current}_MSN \) at least, in the same attributes in which \( \text{Current}_MSN \) is similar to \( Q \), are eliminated from \( T \) (using \( SimArray(\text{Current}_MSN, P_i) \)).

After the Initial approximation and the Eliminating steps, if \( T \) is not empty, the approximation step is performed.

- **Approximating steps.** In this step, a new prototype \( MSN \in T \) is randomly selected, compared against \( Q \), eliminated from \( T \) and used to update the current \( k \) most similar neighbors. If \( \text{Sim}(Q, MSN') < \text{SimThres} \), a new \( MSN' \) is randomly selected (Approximating step). Otherwise, if \( \text{Sim}(Q, MSN') \geq \text{SimThres} \), the prototype \( MSN' \) is used to eliminate prototypes from \( T \) (Eliminating step).

This process is repeated until the set \( T \) is empty. After finding the \( k \) most similar neighbors, the majority class is assigned to \( Q \).
5 LAEMD

The third fast $k$-MSN classifier LAEMD is a modification of AEMD, which aims to reduce the storage space required by AEMD, following the ideas of LAESA (Mico et al., 1994). In the preprocessing phase, LAEMD selects a subset of base prototypes ($BP$) from $T$, and the distances between the prototypes in $T$ and the prototypes in $BP$ are computed and stored in SimArray, which is smaller than SimArray (used in AEDM), since $|BP| << |T|$.

In LAESA, the $BP$ selection consists in finding the farthest prototype in average to the remaining prototypes (not yet selected as $BP$) and this process is repeated until a predefined number ($m$) of $BP$ have been selected.

Since, an important step for the performance of LAESA classifiers is the $BP$ selection algorithm, in this thesis two $BP$ selection algorithms (Hernández-Rodríguez-d et al., 2008) are introduced:

1. **BP selection using class information ($BPClass$)**. In this algorithm, taking advantage of the class information, the $BP$ set is created by selecting roughly the same number of elements from each class, in order to obtain a balanced subset. To select the prototypes for a class, such prototypes which are the most similar, on average, to the rest of the prototypes from the same class are selected; this process is repeated for each class to select the $BP$ set.

2. **BP selection using representative prototypes of the tree TS ($BPNodeTS$)**. In this case, the TS tree structure is used to select some prototypes from the training set. The set of base prototypes ($BP$) is composed by the representative prototypes of the nodes of TS tree. In this case, if the number of nodes in the tree is bigger than $m$, then only the representative prototypes of the first $m$ nodes, found by a breath search, are selected. Breadth search is used, in order to consider the nodes from the first levels of the tree, since the nodes in the first levels of the tree represent more prototypes than nodes in deeper levels.

6 Tree LAEMD

In this section, the proposed fast $k$-MSN classifier Tree LAEMD (Hernández-Rodríguez-e et al., 2008) is introduced. Tree LAEMD is based on a hybrid approach, which uses a tree structure and new Approximating-Eliminating steps, for mixed data and any non metric comparison function. Tree LAEMD consists of two phases: preprocessing and classification.
6.1 Preprocessing phase of Tree LAEMD

In the preprocessing phase, we proposed to compute and store a tree structure, a Boolean tri-dimensional array, a representative prototype per class and a similarity threshold, as follows:

1. **Tree structure (TS)**, which is described in Section 3.1.
2. **Boolean tri-dimensional array (SimArrayNodesTS)**. This array stores the similarity between the representative prototypes of the nodes in TS tree. This array is smaller than the one used in AESA, because the number of nodes in TS tree is smaller than the number of elements in the training set. Besides, this array is used during the classification phase to prune nodes during the tree traversal.

In this case, SimArrayNodesTS[Rep_a,Rep_b,xi]=1, if the representative prototypes Rep_a and Rep_b (of the nodes a and b) are similar regarding the attribute x_i (i=1,…,d, where d is the number of attributes in the prototypes) and otherwise SimArrayNodesTS[Rep_a,Rep_b,xi]=0. In order to evaluate the similarity per attribute between two prototypes, the criteria described in Section 4.1, were used.

3. **Similarity threshold between prototypes (SimThres)**. This value is used during the tree traversal algorithm to decide if a representative prototype of a node of the tree TS can be used to prune nodes in the tree and it is computed as described in Section 4.1.

4. **A representative prototype per class (RP_c)**. These values are computed as described in Section 4.1.

### Preprocessing phase

<table>
<thead>
<tr>
<th>The following is computed:</th>
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<tbody>
<tr>
<td>1. Tree structure (TS)</td>
</tr>
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<td>2. Boolean tri-dimensional array (SimArrayNodesTS)</td>
</tr>
<tr>
<td>3. Similarity threshold between prototypes (SimThres)</td>
</tr>
<tr>
<td>4. Representative prototypes per class (RP_c)</td>
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</tbody>
</table>

### Classification phase

<table>
<thead>
<tr>
<th>New prototype to classify (Q):</th>
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</thead>
<tbody>
<tr>
<td>Initial approximation of the k MSN to Q (using RP_c)</td>
</tr>
<tr>
<td>Tree traversal algorithm to update the k MSN to Q (using TS, SimThres and SimArray)</td>
</tr>
<tr>
<td>Final decision of the class of Q</td>
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</tbody>
</table>

**Figure 3.** General diagram of Tree LAEMD classifier

6.2 Classification phase of Tree LAEMD

In the classification phase, given a new query Q to classify TS, SimThres, SimArrayNodesTS, and RP_c, computed during the preprocessing phase, are used to avoid prototype comparison, as follows:

1. **Initial approximating step.** In this step, the representative prototypes per class (RP_c) are compared against Q to obtain a first approximation of the k most similar neighbors.
2. **Tree traversal step.** In order to update the k most similar neighbors, two algorithms to traverse the tree (Approximating step) are proposed:
• Depth First Search, DFSAE
• Best First Search, BFSAE

During the tree traversal algorithm, if a representative prototype (Rep) of a node is similar enough to Q (Sim(Q,Rep)>SimThres), then all nodes whose representative prototypes are dissimilar to Rep are pruned, using the information about the similarity between representative prototypes stored in SimArrayNodesTS (Eliminating step).

3. Classification step. Finally, the majority class of the k MSN is assigned to Q.

In Figure 3, a general diagram of Tree LAEMD classifier is depicted.

7 Experimental results

In order to evaluate the performance of the proposed classifiers (Tree k-MSN, AEMD, LAEMD and Tree LAEMD), they are compared against the exhaustive k-NN algorithm (Cover & Hart, 1967) and the following tree-based fast k-NN classifiers:

1. Adapted FN classifier (Fukunaga & Narendra, 1975)
2. Adapted GB classifier using GR pruning rule (Gómez-Ballester et al., 2006)
3. Adapted ONC classifier (Oncina et al., 2007)
4. Adapted MS classifier (Moreno-Seco et al., 2003)

To compare FN, GB, ONC and MS classifiers with our proposed fast k-MSN classifier, we adapted these classifiers. The adaptation consisted in the use of the same tree structure (TS) proposed in Section 3.1 and the same function, suitable to work with mixed data, instead of a distance function. In this way, only the search algorithm of the fast k-NN classifiers, is compared.

Besides, since GB tree traversal search algorithm was proposed for a binary tree, in our GR adaptation the pruning rule is applied to all of the C-1 sibling nodes. When a leaf node is reached, as it could contain more than one prototype, a local exhaustive comparison is performed to find the k-MSN.

Since Cluster tree is proposed to work with any dissimilarity, we use this classifier with the same comparison functions for mixed data.

Also, the following Approximating-Eliminating-approach fast k-NN classifiers were compared:
1. AESA classifier (Vidal, 1986)
2. LAESA classifier (Mico et al., 1994), using m=20% of the prototypes in the dataset
3. iAESA classifier (Figueroa et al., 2006)
4. Probabilistic iAESA classifier (Figueroa et al., 2006)

Finally, the following fast k-NN classifiers based on the hybrid-approach were also considered:
1. TLAESA (Mico et al., 1996)
2. Modified TLAESA (Tokoro, 2006)

To compare Approximating-Eliminating and hybrid-approaches, the same comparison function for mixed data was used. In this work, the dissimilarity function HVDM (Wilson & Martinez, 2000), was used for the experiments. This comparison function was selected because it allows comparing mixed data and it is not a metric function since it does not satisfy the triangle inequality property.

For the experiments, 10 datasets from the UCI repository (Blake & Merz, 1998) were used (see Table 2).

In order to compare the different classifiers, the accuracy (Acc) and the percentage of comparisons between prototypes (Comp), were considered. The accuracy was computed as follows:

\[
Acc = \frac{NoCorrectPrototypes \times 100}{NoTestPrototypes} \quad (9)
\]

Where, NoCorrectPrototypes is the number of correctly classified prototypes in the testing set and NoTestPrototypes is the size of the testing set. The percentage of comparisons between prototypes was computed as follows:

\[
Comp = \frac{NoCompFastClassifier \times 100}{NoTrainingPrototypes} \quad (10)
\]

Where NoCompFastClassifier is the number of comparisons done by the fast k-NN classifier, and NoTrainingPrototypes is the size of the training set. According to (10), the exhaustive classifier does the 100% of the comparisons.
In all the experiments ten-fold-cross-validation was used. According to this technique, the dataset is divided in ten partitions; nine of them are used for training and the last partition is used as testing set. This process is repeated ten times, in such a way that each partition is used once as testing set.

In (Hernandez-Rodriguez et al., 2007) different experiments for choosing a value of the parameter C and PercThres were done. In our experiments, C=3, NoP=10% of the dataset, and PercThres=100% were used, since in (Hernandez-Rodriguez et al., 2007), the fast k-NN classifiers reached their best results with these values.

In table 3, the results (Acc and Comp) obtained with the different tree-based fast k-NN classifiers, are shown. From this table, we can notice that the adapted FN, GB and ONC become approximate methods (the classification accuracy is not the same as using the exhaustive k-NN) using HVDM function, which occurs because this comparison function does not satisfy the triangle inequality property. From table 2, we can also notice that Cluster tree, which is the only fast k-NN classifier in the state of the art, proposed to work with non metric functions, reduced more the number of prototype comparisons required to classify a new query (from 100% to 37.18%). However, the classification accuracy was decreased from 81.12% (obtained by k-NN) to 73.57%. From all the tree-based fast k-NN classifiers, ONC obtained the best results (i.e. classification accuracy did not decrease and the percentage of comparisons was reduced from 100% to 36.37%).

In table 4, the results (Acc and Comp) obtained with different Approximating-Eliminating and Hybrid approaches for fast k-NN classifiers, are shown. From this table, we can notice that AESA, LAESA, iAESA, TLAESA and modified TLAESA also become approximate methods, using HVDM function. From table 3, it can also be observed that probabilistic iAESA reduced more the number of prototype comparisons required to classify a new query (from 100%, done by the k-NN to 22.45%).

In table 5, the results obtained with the fast k-MSN classifiers proposed in this work: Tree k-MSN (using DF search to traverse the tree), AEMD, LAEMD (using the algorithm BPNodesTS to select base prototypes), Tree LAEMD (using the DFSAE tree traversal algorithm), are presented. From this table, it is possible to notice that all the proposed classifiers obtained similar
classification accuracy than all the other evaluated methods (enlisted in tables 3 and 4) but achieved a biggest reduction in the number of prototype comparisons. Among the proposed classifiers, Tree LAEMD obtained the best results. Additionally, a t-student test (Dietterich, 1998) with a confidence level of 95%, was done. From this test, we noticed that the classification accuracy difference between the proposed classifiers and all other evaluated fast k-NN classifiers is not statistically significant, while the prototype comparison reduction (done by Tree k-MSN, AEMD, LAEMD and Tree LAEMD) is statistically significant.

Table 4. Classification accuracy (Acc) and percentage of comparisons (Comp), obtained by Approximating-Eliminating and Hybrid-approach fast k-NN classifiers, using HVDM function and k=1 MSN

<table>
<thead>
<tr>
<th>Datasets</th>
<th>AESA Acc</th>
<th>Comp</th>
<th>LAESA Acc</th>
<th>Comp</th>
<th>TLAESA Acc</th>
<th>Comp</th>
<th>Modified TLAESA Acc</th>
<th>Comp</th>
<th>IAESA Acc</th>
<th>Comp</th>
<th>Probabilistic IAESA Acc</th>
<th>Comp</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hepatitis</td>
<td>81,68</td>
<td>51.03</td>
<td>80,61</td>
<td>60.73</td>
<td>81,64</td>
<td>84.64</td>
<td>81,03</td>
<td>68.26</td>
<td>81,64</td>
<td>49.37</td>
<td>80,29</td>
<td>37.85</td>
</tr>
<tr>
<td>Zoo</td>
<td>97,00</td>
<td>21.34</td>
<td>96,00</td>
<td>25.23</td>
<td>95,75</td>
<td>55.77</td>
<td>95,78</td>
<td>27.34</td>
<td>97,20</td>
<td>21.04</td>
<td>95,42</td>
<td>18.56</td>
</tr>
<tr>
<td>Flag</td>
<td>53,60</td>
<td>27.23</td>
<td>52,82</td>
<td>27.57</td>
<td>52,01</td>
<td>49.25</td>
<td>50,19</td>
<td>42.94</td>
<td>52,53</td>
<td>27.15</td>
<td>52,00</td>
<td>25.93</td>
</tr>
<tr>
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<td>82,54</td>
<td>64.34</td>
<td>82,08</td>
<td>67.39</td>
<td>82,25</td>
<td>75.84</td>
<td>82,12</td>
<td>38.30</td>
<td>82,62</td>
<td>63.18</td>
<td>82,34</td>
<td>63.04</td>
</tr>
<tr>
<td>Hayes</td>
<td>83,71</td>
<td>21.23</td>
<td>80,71</td>
<td>21.84</td>
<td>80,73</td>
<td>49.44</td>
<td>80,48</td>
<td>25.49</td>
<td>82,31</td>
<td>21.02</td>
<td>81,84</td>
<td>20.62</td>
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<td>2.07</td>
<td>89,87</td>
<td>5.12</td>
<td>89,87</td>
<td>38.44</td>
<td>87,23</td>
<td>18.35</td>
<td>89,03</td>
<td>2.05</td>
<td>90,23</td>
<td>2.04</td>
</tr>
<tr>
<td>Bridges</td>
<td>63,21</td>
<td>24.23</td>
<td>60,37</td>
<td>26.23</td>
<td>59,37</td>
<td>48.45</td>
<td>59,49</td>
<td>38.92</td>
<td>60,64</td>
<td>24.71</td>
<td>60,60</td>
<td>24.57</td>
</tr>
<tr>
<td>Glass</td>
<td>68,18</td>
<td>13.20</td>
<td>68,18</td>
<td>24.53</td>
<td>68,18</td>
<td>49.54</td>
<td>68,18</td>
<td>22.39</td>
<td>68,18</td>
<td>11.92</td>
<td>67,32</td>
<td>11.25</td>
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<tr>
<td>Iris</td>
<td>94,67</td>
<td>8.23</td>
<td>94,67</td>
<td>10.68</td>
<td>94,67</td>
<td>42.54</td>
<td>94,67</td>
<td>13.29</td>
<td>94,67</td>
<td>8.05</td>
<td>94,00</td>
<td>8.01</td>
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<tr>
<td>Wine</td>
<td>95,46</td>
<td>14.23</td>
<td>95,46</td>
<td>14.75</td>
<td>95,46</td>
<td>46.45</td>
<td>95,46</td>
<td>13.52</td>
<td>95,46</td>
<td>13.58</td>
<td>95,41</td>
<td>12.58</td>
</tr>
<tr>
<td>Avg.</td>
<td>80,99</td>
<td>24.71</td>
<td>80,08</td>
<td>28.41</td>
<td>79,59</td>
<td>53.04</td>
<td>79,46</td>
<td>30.88</td>
<td>80,46</td>
<td>24.21</td>
<td>79,95</td>
<td>22.45</td>
</tr>
</tbody>
</table>

Table 5. Classification accuracy (Acc) and percentage of comparisons (Comp), obtained by the proposed fast k-MSN classifiers, using HVDM function and k=1 MSN

<table>
<thead>
<tr>
<th>Datasets</th>
<th>Tree k-MSN Acc</th>
<th>Comp</th>
<th>AEDM Acc</th>
<th>Comp</th>
<th>LAEDM Acc</th>
<th>Comp</th>
<th>Tree LAEDM Acc</th>
<th>Comp</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hepatitis</td>
<td>81,71</td>
<td>9.54</td>
<td>81,31</td>
<td>14.63</td>
<td>81,64</td>
<td>18.96</td>
<td>81,59</td>
<td>13.23</td>
</tr>
<tr>
<td>Zoo</td>
<td>96,00</td>
<td>19.68</td>
<td>95,10</td>
<td>18.61</td>
<td>97,00</td>
<td>32.85</td>
<td>96,00</td>
<td>12.79</td>
</tr>
<tr>
<td>Flag</td>
<td>52,21</td>
<td>13,20</td>
<td>53,63</td>
<td>16.23</td>
<td>52,00</td>
<td>17,44</td>
<td>52,47</td>
<td>9.73</td>
</tr>
<tr>
<td>Echocard.</td>
<td>79,62</td>
<td>16,50</td>
<td>82,62</td>
<td>17,51</td>
<td>82,62</td>
<td>21,66</td>
<td>81,49</td>
<td>13,05</td>
</tr>
<tr>
<td>Hayes</td>
<td>83,52</td>
<td>18,19</td>
<td>83,85</td>
<td>14,52</td>
<td>83,85</td>
<td>18,42</td>
<td>82,17</td>
<td>10,67</td>
</tr>
<tr>
<td>Soybean-L</td>
<td>85,26</td>
<td>9,72</td>
<td>90,54</td>
<td>11,52</td>
<td>90,54</td>
<td>16,25</td>
<td>89,37</td>
<td>7,83</td>
</tr>
<tr>
<td>Bridges</td>
<td>60,36</td>
<td>15,80</td>
<td>61,85</td>
<td>17,62</td>
<td>60,64</td>
<td>17,96</td>
<td>60,60</td>
<td>8,32</td>
</tr>
<tr>
<td>Glass</td>
<td>67,73</td>
<td>12,91</td>
<td>67,01</td>
<td>14,99</td>
<td>68,18</td>
<td>15,72</td>
<td>68,18</td>
<td>8,38</td>
</tr>
<tr>
<td>Iris</td>
<td>92,67</td>
<td>15,66</td>
<td>94,09</td>
<td>14,82</td>
<td>94,09</td>
<td>15,62</td>
<td>94,67</td>
<td>10,37</td>
</tr>
<tr>
<td>Wine</td>
<td>91,57</td>
<td>13,80</td>
<td>95,00</td>
<td>14,62</td>
<td>95,00</td>
<td>18,51</td>
<td>95,46</td>
<td>12,07</td>
</tr>
<tr>
<td>Avg.</td>
<td>79,27</td>
<td>14,50</td>
<td>80,70</td>
<td>13,50</td>
<td>80,56</td>
<td>19,29</td>
<td>80,20</td>
<td>10,64</td>
</tr>
</tbody>
</table>

In Figure 4, a graph of the accuracy (Acc) against the number of prototype comparisons (Comp) is shown. From this graph, we can notice that all the classifiers obtained similar average classification accuracy, except Cluster tree which obtained the lowest classification accuracy results. However, the proposed classifiers (Tree k-MSN, AEMD, LAEMD and Tree LAEMD), did the smallest number of prototype comparisons. All the experiments were repeated, using k=3 and k=5 and the performance of the fast k-NN classifiers were similar.
8 Conclusions

The development of fast $k$-NN classifiers has been an active research area in the last years, but most of these classifiers rely on metric properties to reduce the number of prototype comparisons. Moreover, very few work has been focused on applications where the comparison function does not satisfy metric properties. For this reason, in this thesis some fast $k$ most similar neighbor ($k$-MSN) classifiers for mixed data and non metric comparisons functions were proposed. To develop these methods, the most successful approaches from the state of the art were followed.

In order to make comparisons, other tree-based fast $k$-NN classifiers were adapted using our proposed tree structure and the same comparison function, to allow them working on mixed data, because of under these circumstances the original algorithms cannot be applied. Also, other methods based on Approximating-Eliminating and Hybrid approaches were considered for comparisons. In these cases, the original algorithms were tested using the same comparison function for mixed data.

Based on our experimental results, in comparison with the exhaustive classifier, and the other fast $k$-NN classifiers (FN, GB, ONC, MS, AESA, LAESA, iAESAs, probabilistic iAESAs, TLAESA, modified TLAESA and Cluster tree), the proposed classifiers (Tree $k$-MSN, AEMD, LAEMD and Tree LAEMD), obtained a big reduction on the number of comparisons between prototypes, which is of particular importance in applications where a fast response is required.

Among the proposed fast $k$-MSN classifiers, using Tree LAEMD the best results were obtained. However, it is important to remark that Tree LAEMD requires more storage space than Tree $k$-MSN. For this reason, the selection of Tree $k$-MSN or Tree LAEMD would depend on the size of the particular problem. The proposed classifier LAEMD is applicable when the comparison function is very expensive, because the preprocessing stage required by LAEMD is faster than the preprocessing stage required by Tree LAEMD.

Finally, we can conclude that for large mixed datasets and non-metric prototype comparison functions, the proposed classifiers are the best option.

As future work, we plan to look for other pruning rules (elimination criteria), not based on metric properties, which would allow us to reduce even more the number of prototype comparisons for AEMD, LAEMD and Tree LAEMD.
References


