Experimental study on prototype optimisation algorithms for prototype-based classification in vector spaces

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Received 13 February 2006; accepted 6 April 2006

Abstract

Prototype-based classification relies on the distances between the examples to be classified and carefully chosen prototypes. A small set of prototypes is of interest to keep the computational complexity low, while maintaining high classification accuracy. An experimental study of some old and new prototype optimisation techniques is presented, in which the prototypes are either selected or generated from the given data. These condensing techniques are evaluated on real data, represented in vector spaces, by comparing their resulting reduction rates and classification performance.

Usually the determination of prototypes is studied in relation with the nearest neighbour rule. We will show that the use of more general dissimilarity-based classifiers can be more beneficial. An important point in our study is that the adaptive condensing schemes here discussed allow the user to choose the number of prototypes freely according to the needs. If such techniques are combined with linear dissimilarity-based classifiers, they provide the best trade-off of small condensed sets and high classification accuracy.

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Keywords: Dissimilarity representation; Prototype selection; Adaptive condensing; EM algorithm; Normal density based classifier; Nearest neighbour rule

1. Introduction

An intuitive way of determining the class of an unknown object is by analysing its similarity to a set of prototypes either selected or generated from a given training set (TS) of objects with known class labels. In general, similarities or dissimilarities can be computed either from the raw object observations or based on an intermediate feature representation. A small set of prototypes has the advantage of a low computational cost and small storage requirements, while leading to similar, or even improved, classification performance. Various ways of designing a prototype set can be studied in Euclidean vector spaces. Two families of such optimisation procedures are editing and condensing.

Editing is the step in a learning process in charge of increasing the accuracy of predictions, when there is substantial noise in the training data. A basic editing algorithm removes noisy instances, as well as close border cases, eliminating a possible overlap between the regions from different classes and leaving smoother decision boundaries. Wilson introduced the first editing method [1]. Briefly, the \( k \)-nearest neighbour (\( k\)-NN) rule is used to estimate the class of each prototype in the TS and to remove those whose class labels do not agree with the ones judged by the \( k\)-NN rule. This algorithm tries to eliminate mislabelled objects from the TS as well as those near to the decision boundaries. Many researchers have addressed the problem of editing by proposing alternative schemes [2–5].

The condensing step aims at selecting a small subset of prototypes without a significant degradation in the classification accuracy. Two main groups of condensing techniques can be distinguished. These are the selective
schemes, which merely select a subset of the original training objects [2,6–9] and the adaptive schemes which modify them [10–15].

This paper discusses prototype optimisation methods, such as editing and condensing, for feature-based representations of classes in the context of prototype-based classification. Traditionally, the 1-NN rule is used for this purpose. It classifies objects based on the minimum distance to the given prototypes. Here, we show that the prototype sets, optimised to guarantee good performance of the 1-NN rule, lead to a higher classification accuracy, when more general dissimilarity-based classifiers are considered, as recently proposed [16,17]. These are weighted linear or quadratic combinations of the (Euclidean) distances computed between the test objects and the prototype sets found by dedicated condensing algorithms. Linear classifiers are especially of interest, since their computational complexity is comparable to that of the 1-NN rule.

Although the algorithms are run in vector spaces, the distances are by no means restricted to the Euclidean metric. Other distances, such as the $l_p$-distances, $d(x,y) = (\sum |x_i - y_i|^p)^{1/p}$, $p > 0$ (metric for $p \geq 1$), or inner-product based distances, $d(x,y) = 1 - \frac{x^T y}{\|x\|\|y\|}$, can be used. Moreover, the selective techniques can easily be applied to non-vectorial data (such as strings, graphs or shapes) provided that the pairwise dissimilarities are derived. This aspect has already been confirmed in earlier studies, in which numerous embeddings of metric and non-metric dissimilarity data (usually derived from non-vectorial representations) were analysed in Euclidean and pseudo-Euclidean spaces [16–18]. There, the prototypes were often chosen at random [18–21]. Other object selection techniques based on feature selection or clustering approaches were studied and appeared to be good for small prototype sets [16,17]. The conclusion of that work is that more general dissimilarity-based classifiers defined by the dissimilarities to a set of selected prototypes are competitive to the NN rule in the context of non-vectorial dissimilarity data.

In this paper we will confirm and extend this conclusion to vectorial representations, where (additionally to selection approaches) adaptive schemes can naturally be applied to create prototypes. These aspects have not been investigated so far. The reason behind our contribution is that the 1-NN (or $k$-NN) rule is often applied in vector spaces\footnote{This holds since the $k$-NN rule is known to be a simple and good classifier for large sample sizes thanks to its theoretical properties [22].} for which editing-and-condensing techniques have been widely studied in order to reduce the computational burden while maintaining high accuracy. Consequently, our paper focusses on vectorial representations and the aspects related to the NN and condensed techniques. It is not our goal to present a general investigation into prototype selection techniques for dissimilarity data resulting from non-vectorial representations; in this case, the reader is referred to Refs. [16,17]. Instead, our goal is to study the applicability of condensing techniques, used in vector spaces to optimise the 1-NN rule, as prototype optimisation techniques for building more general dissimilarity-based classifiers.

We will show that linear or quadratic dissimilarity-based classifiers may successfully replace the 1-NN rule, especially when small sets of prototypes are needed. We will focus on Euclidean distances to maintain the connection with the traditionally used distances for selective condensing schemes in vector spaces. We will also compare these with adaptive reduction algorithms. Consequently, we focus on Euclidean distances in vector spaces and the use of condensing schemes determined in favour of the 1-NN rule. Adaptive schemes are especially of interest, as they can only be used when vectorial representations are available. Consequently, as they offer more flexibility, they should be more beneficial in vector spaces than the selective approaches.

Four condensing techniques are studied. Experiments are conducted to compare their ability to reduce the training size, while maintaining the discriminative power of the optimised prototypes. The classification performance is judged by the 1-NN rule and two more general dissimilarity-based classifiers.

The paper is organised as follows: Section 2 briefly reviews a number of condensing techniques which are used in our study. These are MaxNCN [14,23], Reconsistent [14], LVQ [24] and MixtGauss [15]. Section 3 briefly describes the framework of the prototype-based classification methods used for the evaluation of the derived condensed sets. In Section 4, the data sets are presented and the experiments are described, providing quantitative results and a further discussion. Finally, the main conclusions are summarised in Section 5.

2. Condensing methods to compare

Assume a TS of $N$ instances, $X = \{x_1, x_2, \ldots, x_N\}$, representing $J$ classes, $C = \{c_1, \ldots, c_J\}$. Each instance $x_i$ is a point (a vector) in an $n$-dimensional feature space $\mathcal{R}^n$. A condensed set consists of $r$, $r \ll n$, prototypes, which are either selected or generated from the examples of $X$. They are determined to represent efficiently the distributions of the classes and be well discriminative, when used to classify the training objects. Their cardinality should be sufficiently small to reduce both the storage and evaluation time.

A condensed set is said to be consistent with respect to a TS if the classification error, estimated by assigning all objects from the TS to the classes of their nearest neighbours in the condensed set, is small; see Refs. [3,7]. Therefore, given a set of prototypes representing the class distribution, the classification rate of the TS can be used to measure the consistency of this set. As the consistent condition is maintained, the smaller the number of prototypes in the condensed set, the better the final result is.

Four condensing algorithms are presented below. These are two selective schemes, MaxNCN and Reconsistent, and two adaptive schemes, LVQ and MixtGauss.
2.1. MaxNCN

The so-called surrounding neighbourhood-based rules may be more informative than the distances between them. The so-called surrounding neighbourhood-based rules [23] try to improve the traditional nearest neighbour approach by making use of such information, especially in relation to the training objects which are nearby the decision boundaries. This can be achieved by taking into account not only the proximity of objects to a given input sample but also their symmetrical distribution around it. As a result, the surrounding neighbours of an object \( p \) should satisfy two complementary conditions:

1. Distance criterion: the neighbours should be as close as possible to \( p \).
2. Symmetry criterion: the neighbours should be distributed as homogeneously as possible around \( p \).

Chaudhuri [25] proposed the concept of a nearest centroid neighbourhood (NCN), which can be viewed as a particular realisation of the surrounding neighbourhood. Let \( p \) be a given object whose \( k \)-NCNs (\( k \) nearest centroid neighbours) should be found in a TS. These \( k \) neighbours can be determined by the following iterative procedure:

1. Find the nearest neighbour of \( p \). Choose it as the first NCN, \( q_1 \).
2. Select the \( i \)th NCN, \( q_i \), \( i \geq 2 \), from \( X \) such that the centroid defined by \( q_i \) and the previously selected NCNs, \( q_1, \ldots, q_{i-1} \) is the closest to \( p \).

As designed, the NCN search method is incremental and the objects around a given sample have a geometrical distribution that tends to surround it. Moreover, the region of influence of the NCN is larger than that of the NN, in general. This is illustrated in Fig. 1, where the regions defined by the 4-NCN and the 4-NN are shown for the given point \( p \).

Algorithm 1 MaxNCN

```plaintext
for i = each Prototype(TS) do
    neighbours_number[i] = 0
    neighbour = next_neighbour(i)
    while neighbour.class = \not{i}.class do
        neighbours_vector[i] = ID(neighbour)
        neighbours_number[i]++
        neighbour = next_neighbour(i)
    end while
end for
while Max_neighbours() > 0 do
    Eliminate Neighbours(id_Max_neighbours)
end while
```

The MaxNCN technique is based on the concept of NCN and relies on the NCN search algorithm, as presented above. A set of prototypes is selected from the TS to guarantee their optimal geometrical distribution with respect to their NCNs. The use of the NCN of a given sample can provide local information about the shape of the probability class distribution, which depends on the nature and class of its NCNs, that is, on the nature of the prototypes in its surrounding area.

The rationale behind this approach is that the prototypes belonging to the same class are located in a neighbouring area and can be replaced by a single representative without significantly affecting the original boundaries. The main reason to employ the NCN instead of the NN is to benefit from its properties, i.e. that the NCN covers a bigger region than the NN, and that these neighbours are located in the area of influence around a given sample which is compensated in terms of their geometrical distribution.

Initially, all training objects are considered as prototypes. The algorithm attempts to replace a group of neighbouring prototypes of the same class by a representative. In order to decide which group of prototypes should be replaced, the NCN of each prototype \( p \) in the TS is computed until reaching a neighbour of a class different than the class of \( p \). The prototype with the largest number of NCNs is defined as a representative of its corresponding group. Since this group lies in the area of influence defined by the NCN distribution, consequently, all its members can now be removed from the TS. Next, given the remaining prototypes, the algorithm updates the number of their neighbours (if some were previously eliminated) as belonging to the group of an already existing representative. This is repeated until there is no group of prototypes to be replaced by a representative. This basic scheme is called MaxNCN, and is presented in Algorithm 1.
Algorithm 2 Reconsistent

for $i = \text{each}_\text{prototype}(TS)$ do
    neighbours_number[$i$] = 0
    neighbour = next_neighbour($i$)
    while neighbour.class = $= i$.class do
        neighbours_vector[$i$] = id(neighbor)
        neighbours_number[$i$] +=
        neighbour = next_neighbour($i$)
    end while
end for

while Max_neighbours() > 0 do
    EliminateNeighbours(id_Max_neighbours)
end while

for $i = \text{each}_\text{prototype}(TS)$ do
    count = 0
    if Classify($i$)! = $i$.class then
        incorrect_class[count + +] = $i$
    end if
end for

for $i = \text{each}_\text{prototype}(\text{incorrect}_\text{class}())$ do
    neighbours_number_inc[$i$] = 0
    neighbour_inc = next_neighbour_inc($i$)
    while neighbour_inc.class = $= i$.class do
        neighbours_vector_inc[$i$] = id(neighbor_inc)
        neighbours_number_inc[$i$] +=
        neighbour_inc = next_neighbour_inc($i$)
    end while
end for

while Max_neighbours_inc() > 0 do
    EliminateNeighbours_inc(id_Max_neighbours_inc)
end while

AddCondensedIncToCondensedTS()

2.2. Reconsistent

The Reconsistent algorithm is an important modification of the MaxNCN algorithm towards obtaining a consistent condensed set [14]. The primary idea is that the consistency of a subset with respect to the TS should lead to a better classification. By using the MaxNCN algorithm some prototypes close to the decision boundaries are removed because of the order in which the instances are taken during the condensing process. The Reconsistent approach, proposed by us, tries to address this issue.

The procedure starts by applying the MaxNCN technique to a TS, yielding a reduced set, RS. Then, each object in the TS is tested by the 1-NN rule with respect to the current prototype set, RS. All misclassified objects form a new group, which is condensed using the RS set as the reference. In the end, this new condensed set is added to the RS, resulting in the final condensed set. The Reconsistent procedure is presented in Algorithm 2.

2.3. LVQ

In statistical pattern recognition, learning vector quantisation (LVQ) is a popular competitive learning algorithm, used in many applications. Its goal is to approximate the distribution of classes by using a reduced set of prototypes, while minimising the classification error [13]. It is, therefore, an adaptive condensing technique. In general, the classes can be described by a relatively small number of prototypes $p_i$, placed within each class region of the decision boundary by means of measures of neighbourhood.

In the initialisation step, the prototypes are placed in the TS, maintaining the same number of prototypes in each class. The class borders are represented in a piecewise linear way by segments of midplanes between the prototypes of neighbouring classes (the borders of the so-called Voronoi tessellations). This may seem to be a good strategy for approximating the class borders, using the fact that the average distances between the neighbouring prototypes should be the same on both sides of the borders.

Nevertheless, the optimal placement of the prototypes is not known. Therefore, their distances and their optimal cardinality, $k$, cannot be determined beforehand. To fix the value of $k$ for each case, the number of prototypes has to be chosen first. A combination of editing and condensing is used for this purpose. Therefore, first the Wilson’s editing ($k$ of the $k$-NN used in the editing scheme, as explained in Section 4.1) is used, and then followed by the Hart’s condensing algorithm [7]. The resulting size of the prototype set is close to ideal [4]. Using this number of prototypes, different values of $k$ were tested, and the one leading to the highest classification accuracy was finally chosen. Different set sizes were used for each data set, in order to compare the results for different cases.

In the experiments, a variant of the original LVQ algorithm is used, namely the optimised-learning-rate, OLQV[1, 24]. The basis of this algorithm is the LVQ1 [24] such that an individual learning rate $\alpha_i(t)$ is selected for each prototype $p_i$. Several prototypes are assigned to each class such that the layout of the prototypes minimise approximately the misclassification errors in the 1-NN classification. The following equations define this process:

$$p_i(t + 1) = p_i(t) + \alpha_i(t)[x(t) - p_i(t)]$$

if $x$ and $p_i$ are in the same class,

$$p_i(t + 1) = p_i(t) - \alpha_i(t)[x(t) - p_i(t)]$$

if $x$ and $p_i$ are in different classes,

$$p_i(t + 1) = p_i(t) \text{ if } i \neq c,$$

where $x(t)$ is an input sample and $p_i$ is the nearest $p_i$ to $x$. In Ref. [24], the “optimal” values of $\alpha_i(t)$ are determined by recursion as

$$\alpha_i(t) = \frac{\alpha_i}{1 + s(t)\alpha_i(t - 1)},$$

where $s(t)$ is the number of correct classification. In general, the classes include a relatively small number of prototypes $p_i$, placed within each class region of the decision boundary by means of measures of neighbourhood.
where \( s(t) = +1 \) if the classification of the prototype \( p_c \) is correct and \( s(t) = -1 \) if the classification is wrong. Therefore, it is necessary to stop the learning process after some “optimal” number of steps. Typically, the OLVQI may be stopped after 200 iterations.

### 2.4. MixtGauss

MixtGauss is an adaptive condensing algorithm proposed by some of us in Ref. [15]. It is considered in the framework of mixture modelling by Gaussian distributions, while assuming a statistical independence of features. The prototypes are chosen as the mean vectors of the optimised Gaussians, whose mixtures are fit to model each of the classes. The details are given below.

In general, given a TS, we assume that each class follows a spatial distribution according to its class-conditional probability density function (pdf) \( P(x|c_j) \) and the respective a priori probability \( P(c_j) \), \( c_j \in C \). These class-conditional pdfs do not need to have a specific structure, in general. In practice, however, it is necessary to obtain their density estimations.

A natural way to deal with a density estimator is to consider a mixture density of modes. One approach to obtain the capacity of \( P(x|c_j) \) is by reflecting the local structure of the distribution by means of mixture modes \( P_m(x|c_j) \), where each mode is estimated by the product of probabilities in each feature as [26]:

\[
P(x|c_j) = \sum_{m=1}^{M} z_{m|j} P_m(x|c_j)
\]

\[
= \sum_{m=1}^{M} z_{m|j} \prod_{k=1}^{n} N(x_k; \mu_m[kj], \sigma_m[kj]),
\]

where \( M \) is the number of modes and \( z_{m|j} \) is a priori probability of the \( m \)th mode in the class \( c_j \).

In our condensing algorithm, each class in the TS is modelled by a probability distribution. A general shape of classes as well as the decision boundaries is maintained, when each class is described by a mixture of multivariate Gaussian distributions. By our additional assumption of the statistical independence of features, the \( m \)th component in a mixture modelling the class \( c_j \) is a multivariate Gaussian distribution expressed by a product of univariate normal distributions, \( N(\mu_m[kj], \sigma_m[kj]) \). Note that this is equivalent to a multivariate elliptic Gaussian distribution \( N(\mu_{m|j}, \text{diag}(\sigma_{m|j})) \). The standard method used to fit finite mixture models to the observed data, hence to estimate the parameters of the class distributions, is the well-known EM algorithm [27,28]. This is a general maximum likelihood optimisation procedure for problems with hidden variables or missing data [29]. The final prototypes of the sought condensed set are the mean vectors of the Gaussian distributions determined by the EM algorithm.

Note that, although the EM algorithm is widely used, one needs to be aware of its drawbacks [30]. As a method working in local neighbourhoods, it is sensitive to initialisation, as the likelihood function of a mixture model is not unimodal. Another important problem in mixture modelling is the selection of the number of components. With too many components, the mixture may overfit the data, while a mixture with too few components may not be flexible enough to approximate the true underlying model.

#### Algorithm 3 MixtGauss

(* initialisation *)

\[
\text{for } c = 1..\text{number of classes do}
\]

\[
\text{mean}[c] = \text{Calculate Mean}(c, T S)
\]

\[
\text{for } g = 1..\text{number of Gaussians per class do}
\]

\[
\text{Gaussians}[c, g] = \text{mean}[c] + \text{Random Disturbance}()
\]

\[
\text{end for}
\]

\[
\text{end for}
\]

(* optimisation *)

\[
\text{repeat}
\]

\[
\text{for } c = 1..\text{number of classes do}
\]

\[
\text{if current accuracy}[c] > \text{previous accuracy}[c] \text{ then}
\]

\[
\text{classes improve} = \text{classes improve} + 1
\]

\[
\text{else}
\]

\[
\text{if current accuracy}[c] > \text{previous accuracy}[c] \text{ then}
\]

\[
\text{Gaussians}[c, g] = \text{previous Gaussians}[c, g]
\]

\[
\text{end for}
\]

\[
\text{end if}
\]

\[
\text{end for}
\]

\[
\text{until classes improve} = 0
\]

#### 2.4.1. Algorithm details

The more Gaussian components are included in a mixture, the more accurate the representation of the classes and the decision boundaries is. Taking this into account, \( M \) Gaussians have to be specified to represent each class distribution. This number corresponds to the number of prototypes generated in each class for the final condensed set. Initially, each class is represented by \( M \) Gaussians located at the mean of that class. By adding random disturbances, different mean vectors are created and the Gaussians are shifted away. So, a mixture of Gaussians can be obtained per class. For each Gaussian, the initial variance is set up to \( \frac{1}{10} \) of the range in each dimension.

After the initialisation stage, the EM algorithm is used to determine an optimal location of the mixture of Gaussians. This iterative optimisation procedure converges to a
maximum likelihood estimate of the mixture parameters. Accordingly, to fit a mixture of Gaussians to each class, we iterate between the following two steps:

E-step: Compute the contributions of the prototypes $x^t$ in the class $c_j$, belonging to the set $\{x^1, \ldots, x^{N_j}\}$, where $N_j$ is the cardinality of the class $c_j$. The conditional pdf for the $m$th mode is

$$P_m(x^t|c_j) = \frac{x_{mj}^{c_j}}{\sum_{l=1}^{M} x_{lj}^{c_j}} \prod_{k=1}^{l} N(x^t_k; \mu_{lk|j}, \sigma_{lk|j})$$

and it is normalised such that $\sum_{m=1}^{M} x_{mj}^{c_j} = 1$. The multivariate Gaussians are represented as a product of univariate normal distributions, with the means $\mu_{lk|j}$ and the standard deviations $\sigma_{lk|j}$.

M-step: Compute the parameters of the $m$th mode for each value $x^t$ that exists in the class $c_j$:

$$x_{mj}^{c_j} = \frac{1}{N_j} \sum_{t=1}^{N_j} P_m(x^t|c_j),$$
$$\mu_{lk|j} = \frac{\sum_{t=1}^{N_j} P_m(x^t|c_j) x^t_k}{\sum_{t=1}^{N_j} P_m(x^t|c_j)},$$
$$\sigma_{lk|j} = \frac{\sum_{t=1}^{N_j} P_m(x^t|c_j) (x^t_k - \mu_{lk|j})^2}{\sum_{t=1}^{N_j} P_m(x^t|c_j)}.$$  \hspace{1cm} (4)

The EM iterative optimisation can cause an overlap between the Gaussian components from different classes, which will deteriorate the final classification accuracy. Therefore, this process should stop when no class yields an increase in performance with respect to the previous iteration. To address this problem, the consistency criterion is applied. After each iteration, the consistency criterion is estimated by calculating the 1-NN error over the TS by using the estimated means of the Gaussians as the current condensed set. The movement of the Gaussians is carried out while any class improves the classification rate with respect to the previous step. The complete technique is summarised in Algorithm 3.

3. Prototype-based classification methods to compare

The usefulness of condensed sets, optimised by the approaches discussed above, will be evaluated in a classification task. Traditionally, the 1-NN rule, assigning an unknown object to the class of its nearest neighbour in the condensed set, is used for this purpose. The 1-NN rule is employed, as it is often used in condensing schemes for the design of the condensed set. If the classes are represented as compact Gaussian-like clouds of similar spreads, then the 1-NN is expected to generalise well for a small condensed set. Otherwise, a large condensed set might be needed to represent the variability in the data. Alternatively, classifiers in the so-called dissimilarity spaces can be considered.

3.1. Dissimilarity spaces

Remember that a TS $X$ consist of $N$ objects in a feature vector space. Let $R = \{x_1, x_2, \ldots, x_r\}$ be a condensed set, called also representation set, of $r$ optimised prototypes. A dissimilarity measure\(^2\) $d$, one may consider a new representation based on the proximities to the set $R$. Every object $x \in X$ is then described by a vector of dissimilarities computed between $x$ and the prototypes from $R$, i.e. $D(x, R) = [d(x, p_1), d(x, p_2), \ldots, d(x, p_r)]$. Hence, for a set $X$, it extends to an $N \times r$ dissimilarity matrix $D(X, R)$.

The dissimilarity matrix $D(X, R)$ is interpreted as a data-dependent mapping $D(\cdot, R) : X \rightarrow \mathbb{R}^r$ from the representation $X$ to a dissimilarity space, defined by the set $R$. This is a vector space, in which each dimension corresponds to a dissimilarity to a prototype from $R$, $D(\cdot, p_1)$. The advantage of this representation is that any traditional classifier operating in vector spaces can now be used [20,16,17].

A vector $D(\cdot, p_1)$ of dissimilarities to the prototype $p_1$ can be interpreted as a feature. This follows since the dissimilarities to other prototypes $p_i$ will differ depending on the class membership. If the measure is metric and the dissimilarity $d(p_1, p_2)$ is small, then $d(x, p_1) \approx d(x, p_2)$ for other object $x$, as it is guaranteed by the backward triangle inequality [17]. As a result, only one of them can be chosen as a prototype. However, a small number of prototypes might be insufficient to represent the data variability if the classes have different spreads (in terms of the dissimilarities). This occurs when, in a feature space one class is represented by a compact cloud of points, while the other class is elongated. It can be, therefore, more beneficial to inspect the vectors of dissimilarities to the entire set $R$, instead of looking at the nearest neighbour only. If the objects $x$ and $y$ are similar, then their dissimilarity vectors $D(x, R)$ and $D(y, R)$ are expected to be correlated. Hence they should lie close in a dissimilarity space (as measured e.g. by an Euclidean distance in this space). A linear or quadratic classifier in this dissimilarity space might be of interest.

3.2. Normal-density based classifiers in dissimilarity spaces

In the case of small condensed sets or non-representative TS, a better generalisation can be achieved by a classifier built in a dissimilarity space than by the 1-NN rule. Many traditional classifiers can be applied there [19–21,17]. Linear and quadratic functions are weighted linear (quadratic) combinations of the dissimilarities $d(x, p_i)$ between a given object $x$ and the prototypes $p_i$. Although the classifiers are trained on $D(\cdot, R)$, the weights are still optimised on the complete TS.

\(^2\) In general, a non-negative dissimilarity measure should express a degree of commonality between pairs of objects. It should be zero for two identical objects, take small values for similar objects and large values for objects that differ. It does not need to be metric.
Bayesian classifiers, i.e. linear and quadratic normal density-based classifiers, tend to perform well in dissimilarity spaces [19,18,20,21,31]. This is especially true, for a summation-based dissimilarity measure, summing over a number of components with similar variances. The reason is that such dissimilarities will be approximately normally distributed thanks to the central limit theorem (if one or few variances are dominant, then they will approximate the \( \chi^2 \) distribution) [17]. In our case, the vectorial data will be normalised to unit variances, hence the resulting Euclidean distances tend to be approximately normally distributed.

One may, therefore, expect a good performance of such decision rules, if the problem is linearly or quadratically separable. Since in our case the Euclidean distance is a non-linear transformation normalised features, a linear classifier in the underlying (original) space [17], similarly to the reasoning for support vector machines [32]. So, if the Euclidean distance is informative for the classification problem in a feature vector space, the local and non-linear 1-NN rule in this space may be replaced by a linear classifier in the Euclidean-distance dissimilarity space.

For a two-class problem, a linear normal density based classifier (NLC), defined by the condensed set dissimilarity space, may be replaced by a linear classifier in the Euclidean-distance dissimilarity space. The local and non-linear 1-NN rule in this space may be informative for the classification problem in a feature vector space. Therefore, as a general rule, the Euclidean distance is a non-linear classifier in the underlying (original) space [17], similarly to the reasoning for support vector machines [32].

The results are compared in terms of both accuracy and reduction of theTS size. The four condensing algorithms are the ones described before: MaxNCN, Reconsistent, LVQ and MixtGauss. The first classification method is the 1-NN rule based on the set \( R \). The other two methods are the FLD and NQC trained in dissimilarity spaces \( D(X, R) \).

### 4. Experimental results and discussion

We will compare some methods of determining a condensed set \( R \) in combination with three prototype-based classification strategies. These are done on Euclidean distance representations \( D(X, R) \) derived in feature spaces. The four condensing algorithms are the ones described before: MaxNCN, Reconsistent, LVQ and MixtGauss. The first classification method is the 1-NN rule based on the set \( R \). The other two methods are the FLD and NQC trained in dissimilarity spaces \( D(X, R) \).

#### 4.1. Data description and experimental setup

Eleven real data sets (see Table 1) are taken from the UCI Repository [35] to assess the behaviour of the algorithms presented here. All data sets are first normalised by a unit variance, and then the Euclidean distances are computed. The results are compared in terms of both accuracy and reduction of theTS size.

<table>
<thead>
<tr>
<th>Data set</th>
<th>No. classes</th>
<th>No. features</th>
<th>TS size</th>
<th>Test set size</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer</td>
<td>2</td>
<td>9</td>
<td>546</td>
<td>137</td>
</tr>
<tr>
<td>Diabetes</td>
<td>2</td>
<td>8</td>
<td>614</td>
<td>154</td>
</tr>
<tr>
<td>Glass</td>
<td>6</td>
<td>9</td>
<td>171</td>
<td>43</td>
</tr>
<tr>
<td>Heart</td>
<td>2</td>
<td>13</td>
<td>216</td>
<td>54</td>
</tr>
<tr>
<td>Liver</td>
<td>2</td>
<td>6</td>
<td>276</td>
<td>69</td>
</tr>
<tr>
<td>Vehicle</td>
<td>4</td>
<td>18</td>
<td>677</td>
<td>169</td>
</tr>
<tr>
<td>Vowel</td>
<td>11</td>
<td>10</td>
<td>422</td>
<td>106</td>
</tr>
<tr>
<td>Wine</td>
<td>3</td>
<td>13</td>
<td>142</td>
<td>36</td>
</tr>
<tr>
<td>Phoneme</td>
<td>2</td>
<td>5</td>
<td>4323</td>
<td>1080</td>
</tr>
<tr>
<td>Satimage</td>
<td>6</td>
<td>36</td>
<td>5148</td>
<td>1287</td>
</tr>
<tr>
<td>Texture</td>
<td>11</td>
<td>40</td>
<td>4400</td>
<td>1100</td>
</tr>
</tbody>
</table>

A multi-class FLD is derived in the one-against-all strategy [33].

#### 4.2. Quantitative results

Tables 2–4 report the classification accuracy of the I-NN, the FLD and the NQC, respectively, obtained by
Table 2
Classification accuracy of the 1-NN (in %)

<table>
<thead>
<tr>
<th>Class</th>
<th>Original</th>
<th>MaxNCN</th>
<th>Reconsistent</th>
<th>LVQ</th>
<th>MixGauss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer</td>
<td>95.2</td>
<td>92.0 [95.2]</td>
<td>93.4 [93.8]</td>
<td>96.9 [99.3]</td>
<td>96.5 [99.3]</td>
</tr>
<tr>
<td>Diabetes</td>
<td>70.1</td>
<td>67.7 [87.0]</td>
<td>71.8 [81.8]</td>
<td>76.6 [98.1]</td>
<td>75.0 [91.9]</td>
</tr>
<tr>
<td>Glass</td>
<td>69.7</td>
<td>64.1 [59.1]</td>
<td>69.4 [46.8]</td>
<td>72.6 [71.9]</td>
<td>64.5 [75.4]</td>
</tr>
<tr>
<td>Heart</td>
<td>76.3</td>
<td>69.3 [83.8]</td>
<td>74.8 [77.8]</td>
<td>84.1 [89.8]</td>
<td>81.9 [93.5]</td>
</tr>
<tr>
<td>Liver</td>
<td>62.6</td>
<td>58.9 [76.8]</td>
<td>61.0 [68.5]</td>
<td>65.6 [93.5]</td>
<td>63.7 [97.1]</td>
</tr>
<tr>
<td>Vehicle</td>
<td>69.4</td>
<td>64.4 [60.3]</td>
<td>66.0 [49.2]</td>
<td>72.2 [61.6]</td>
<td>69.6 [70.5]</td>
</tr>
<tr>
<td>Vowel</td>
<td>98.1</td>
<td>90.8 [74.4]</td>
<td>95.5 [71.8]</td>
<td>80.8 [76.5]</td>
<td>90.7 [76.5]</td>
</tr>
<tr>
<td>Wine</td>
<td>94.4</td>
<td>91.6 [93.0]</td>
<td>92.1 [90.9]</td>
<td>95.5 [95.8]</td>
<td>96.0 [97.9]</td>
</tr>
<tr>
<td>Phoneme</td>
<td>71.0</td>
<td>69.1 [91.6]</td>
<td>70.2 [88.9]</td>
<td>77.3 [93.1]</td>
<td>73.3 [93.1]</td>
</tr>
<tr>
<td>Satimage</td>
<td>83.0</td>
<td>79.2 [86.5]</td>
<td>80.3 [82.7]</td>
<td>82.2 [88.3]</td>
<td>81.3 [94.8]</td>
</tr>
<tr>
<td>Texture</td>
<td>98.9</td>
<td>95.3 [89.3]</td>
<td>97.3 [87.8]</td>
<td>85.9 [99.5]</td>
<td>97.2 [90.0]</td>
</tr>
<tr>
<td>Average</td>
<td>80.8</td>
<td>76.6 [81.5]</td>
<td>79.2 [76.4]</td>
<td>80.9 [87.9]</td>
<td>80.9 [89.1]</td>
</tr>
</tbody>
</table>

The corresponding reduction rates of the TS size (in %) and the equivalent number of prototypes are given in brackets.

Table 3
Classification accuracy of the FLD in dissimilarity spaces (in %)

<table>
<thead>
<tr>
<th>Class</th>
<th>Original</th>
<th>MaxNCN</th>
<th>Reconsistent</th>
<th>LVQ</th>
<th>MixGauss</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Cancer</td>
<td>85.50</td>
<td>96.48 [95.2]</td>
<td>96.48 [93.8]</td>
<td>97.22 [98.2]</td>
<td>96.92 [96.3]</td>
</tr>
<tr>
<td>2 Diabetes</td>
<td>74.23</td>
<td>76.05 [87.0]</td>
<td>77.09 [81.8]</td>
<td>77.08 [98.7]</td>
<td>76.70 [87.0]</td>
</tr>
<tr>
<td>3 Glass</td>
<td>53.88</td>
<td>66.53 [59.1]</td>
<td>67.49 [46.8]</td>
<td>77.17 [61.4]</td>
<td>69.77 [93.0]</td>
</tr>
<tr>
<td>4 Heart</td>
<td>60.75</td>
<td>80.72 [83.8]</td>
<td>78.49 [77.8]</td>
<td>84.79 [98.1]</td>
<td>82.60 [98.2]</td>
</tr>
<tr>
<td>5 Liver</td>
<td>68.35</td>
<td>68.96 [76.8]</td>
<td>67.83 [68.5]</td>
<td>70.70 [92.8]</td>
<td>68.67 [93.5]</td>
</tr>
<tr>
<td>6 Vehicle</td>
<td>77.19</td>
<td>79.31 [60.3]</td>
<td>79.79 [49.2]</td>
<td>80.96 [67.5]</td>
<td>80.02 [76.4]</td>
</tr>
<tr>
<td>7 Vowel</td>
<td>41.03</td>
<td>95.76 [74.4]</td>
<td>96.67 [71.8]</td>
<td>91.42 [76.5]</td>
<td>94.28 [76.5]</td>
</tr>
<tr>
<td>8 Wine</td>
<td>33.15</td>
<td>98.28 [93.0]</td>
<td>98.30 [90.9]</td>
<td>98.87 [95.8]</td>
<td>98.90 [95.8]</td>
</tr>
<tr>
<td>9 Phoneme</td>
<td>70.62</td>
<td>69.75 [91.6]</td>
<td>70.52 [88.9]</td>
<td>77.11 [98.2]</td>
<td>73.94 [99.8]</td>
</tr>
<tr>
<td>10 Satimage</td>
<td>24.49 [86.5]</td>
<td>23.90 [82.7]</td>
<td>82.11 [95.3]</td>
<td>82.20 [95.9]</td>
<td>82.20 [95.9]</td>
</tr>
<tr>
<td>Average (1–11)</td>
<td>72.2 [81.5]</td>
<td>71.3 [76.4]</td>
<td>85.1 [88.6]</td>
<td>83.9 [91.5]</td>
<td>82.4</td>
</tr>
<tr>
<td>Average (1–9)</td>
<td>62.7</td>
<td>81.3</td>
<td>81.4</td>
<td>83.9</td>
<td>82.4</td>
</tr>
</tbody>
</table>

The corresponding reduction rates of the TS size (in %) are given in brackets. Averages over all data sets (1–11) and data sets excluding Satimage and Texture (1–9), are also given.

Table 4
Classification accuracy of the NQC in dissimilarity spaces (in %)

<table>
<thead>
<tr>
<th>Class</th>
<th>Original</th>
<th>MaxNCN</th>
<th>Reconsistent</th>
<th>LVQ</th>
<th>MixGauss</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cancer</td>
<td>80.23</td>
<td>96.19 [95.2]</td>
<td>96.48 [93.8]</td>
<td>97.22 [96.3]</td>
<td>96.34 [96.3]</td>
</tr>
<tr>
<td>Diabetes</td>
<td>65.62</td>
<td>75.39 [87.0]</td>
<td>74.74 [81.8]</td>
<td>77.09 [97.1]</td>
<td>76.70 [98.7]</td>
</tr>
<tr>
<td>Glass</td>
<td>40.15</td>
<td>53.81 [59.1]</td>
<td>54.40 [46.8]</td>
<td>65.10 [89.5]</td>
<td>64.11 [82.5]</td>
</tr>
<tr>
<td>Heart</td>
<td>55.56</td>
<td>82.97 [83.8]</td>
<td>80.00 [77.8]</td>
<td>82.95 [97.2]</td>
<td>82.21 [88.9]</td>
</tr>
<tr>
<td>Liver</td>
<td>46.67</td>
<td>62.63 [76.8]</td>
<td>60.00 [68.5]</td>
<td>67.79 [85.5]</td>
<td>65.20 [89.1]</td>
</tr>
<tr>
<td>Vehicle</td>
<td>27.78</td>
<td>60.27 [60.3]</td>
<td>54.37 [49.2]</td>
<td>74.81 [76.4]</td>
<td>74.58 [91.1]</td>
</tr>
<tr>
<td>Vowel</td>
<td>10.20</td>
<td>31.96 [74.4]</td>
<td>29.41 [71.8]</td>
<td>94.59 [92.2]</td>
<td>94.10 [92.2]</td>
</tr>
<tr>
<td>Wine</td>
<td>33.15</td>
<td>97.73 [93.0]</td>
<td>96.05 [90.9]</td>
<td>97.76 [97.9]</td>
<td>99.43 [95.8]</td>
</tr>
<tr>
<td>Phoneme</td>
<td>73.26</td>
<td>73.08 [91.6]</td>
<td>73.22 [88.9]</td>
<td>76.11 [95.4]</td>
<td>73.33 [95.4]</td>
</tr>
<tr>
<td>Satimage</td>
<td>79.40 [86.5]</td>
<td>79.17 [82.7]</td>
<td>81.93 [98.3]</td>
<td>81.62 [97.1]</td>
<td>81.62 [97.1]</td>
</tr>
<tr>
<td>Texture</td>
<td>96.31 [89.3]</td>
<td>96.51 [87.8]</td>
<td>97.58 [95.0]</td>
<td>97.53 [96.3]</td>
<td>97.53 [96.3]</td>
</tr>
<tr>
<td>Average (1–11)</td>
<td>73.6 [81.5]</td>
<td>72.2 [76.4]</td>
<td>83.0 [92.8]</td>
<td>82.3 [93.0]</td>
<td>80.7</td>
</tr>
<tr>
<td>Average (1–9)</td>
<td>48.1</td>
<td>70.5</td>
<td>68.7</td>
<td>81.5</td>
<td>80.7</td>
</tr>
</tbody>
</table>

The corresponding reduction rates of the TS size (in %) are given in brackets. Averages over all data sets (1–11) and data sets excluding Satimage and Texture (1–9), are also given.

using different condensed sets. For each condensing method, the average performance values, computed over the 11 data sets are also included. There are no results of the FLD and the NQC for the Satimage and Texture sets (for the original TS), because of their high memory requirements during training [33]. The average performances excluding these
The first observation is that the LVQ and the MixtGauss increase the average accuracy in comparison to the original TS accuracy. The increase is larger by using the FLD and the NQC than by using the 1-NN rule (where the increase is quite small). Anyway, it is significant that in all these cases, the performance is increased despite the high reduction of the TS (see Tables 2–4). Remember that although the FLD and the NQC are based on the distances to the prototypes, they still make use of the entire TS in training. This is the reason why the classification accuracy increases so much when using any condensed set, in comparison to the results by using the original TS.

By using the FLD, the classification accuracy obtained for the MaxNCN and Reconsistent procedures is very similar. The MixtGauss leads to a higher accuracy than both of them. The best performance of the FLD relies on the LVQ. A similar pattern can be observed for the NQC. This differs, however, for the 1-NN rule, especially in the case of the Reconsistent algorithm. The smallest classification accuracy is reached for the MaxNCN. The Reconsistent gives better results, and the best values are obtained for the LVQ and the MixtGauss.

The training reduction rates, being the percentage by which the original training size is reduced, are provided in square brackets in Tables 2–4. Since the MaxNCN and the Reconsistent techniques determine the optimal number of prototypes directly, their reduction rates are identical for the three classification methods used. Additionally, for each condensing method, the average reduction values computed over the 11 data sets are also included.

In relation to the training reduction rates, the average is higher for the MaxNCN than for the Reconsistent. This is
to be expected as in the second algorithm, some instances are added to the MaxNCN condensed set to improve the classification accuracy. It can also be observed that the average TS reduction rates are higher for the adaptive LVQ and MixtGauss techniques than for the selective MaxNCN and Reconsistent procedures. The highest reduction rate is the one of MixtGauss. This holds for the three prototype-based classification strategies used here.

In relation to the classification methods considered, in general, we can observe that the FLD and the NQC perform better than the 1-NN rule, when they rely on the condensed sets determined by the adaptive schemes. Comparing both algorithms, the one with the best performance corresponds to the FLD. On the other hand, the MaxNCN and the Reconsistent procedures have their best classification accuracy with the 1-NN rule. As designed, the Reconsistent leads to a higher nearest neighbour performance than the MaxNCN.

These results can be better analysed by studying the graphs for each data set (see an example for four data sets in Fig. 2). The best trade-off results (between the accuracy and the reduced TS size) are the ones for the FLD. The results for the NQC are similar, and the ones for the 1-NN rule are significantly worse. In relation to the condensing algorithms, the LVQ and the MixtGauss lead to very similar results. In general, the points corresponding to the MaxNCN-FLD and the Reconsistent-FLD results are near the functions representing the MixtGauss-FLD and the LVQ-FLD results, similarly as the points representing the MaxNCN-NQC and the Reconsistent-NQC results are close to the points describing the MixtGauss-NQC and the LVQ-NQC results. This observation does not hold for the MaxNCN-NN and the Reconsistent-NN, neither the MixtGauss-NN and the LVQ-NN, as there exists a big difference in favour of the MixtGauss and the LVQ for some data sets.

In Fig. 2, the behaviour of the algorithms investigated here is shown for four data sets. Only the results for the smallest reduced sets for each data are plotted, in order to distinguish the plots. The first graph, Fig. 2(a), refers to the Vehicle data set. It can be observed that the best classification accuracy is reached by the MixtGauss-NQC for the smallest condensed sets. For sets with more than three instances per class, the best accuracy is reached by the LVQ-FLD. It is to note that the performance of the MixtGauss-FLD is always close to the best case.

In Fig. 2(b) the results for the Vowel data set are shown. The three smallest condensed sets represented (1, 2 and 3 instances per class) lead to the best performance for the combination of the LVQ-NQC and the MixtGauss-NQC algorithms. However, for larger sizes, the classification accuracy suddenly decreases. It is due to a large number of classes in relation to the number of prototypes, which effectively translates into the dimension of the dissimilarity space. As a result, the number of instances per class is too small, and as the size of the condensed set increases, class covariance matrices are badly estimated. Hence, the classification accuracy is diminished. The next best results belong to the MixtGauss-FLD, the LVQ-FLD and the MixtGauss-NN, in that order.

In Fig. 2(c), the results for the Satimage data set are shown. The most reduced sets lead to a better performance by using the MixtGauss-NQC, the LVQ-NQC, the MixtGauss-FLD and the LVQ-FLD methods. The results for the data set Texture are shown in Fig. 2(d). The best ones are obtained by the following combinations: the LVQ-NQC, the MixtGauss-NQC, the LVQ-FLD and the MixtGauss-FLD. As it is not plotted in this paper, in order to save space, it could be important to know the next point. The larger graphs for Satimage and Texture data sets show that the classification accuracy also decreases around the size of 300 instances for the MixtGauss-FLD and the LVQ-FLD. It is due to similar reasons as mentioned for the Vowel data.

5. Conclusions

This paper compares several prototype reduction techniques, including both selecting and generating schemes, in connection with performance of classifiers defined on the corresponding sets of prototypes. We use the following classifiers: the 1-NN rule, and linear and quadratic prototype-based classifiers defined in Euclidean-distance dissimilarity spaces. The purpose of this experimental study is to discuss a number of prototype optimisation methods with respect to their ability of maintaining small prototype sets and high classification performance.

From our investigations it can be concluded that there is no significant difference between the LVQ and the MixtGauss prototype generation techniques. However, when comparing them to the MaxNCN and Reconsistent methods, the first two algorithms tend to give both larger reduction of the TS (i.e. smaller condensed sets) and lead to higher classification accuracy. This means that the LVQ and the MixtGauss are good as condensing algorithms since they yield a good performance and allow one to control the number of prototypes. Additionally, they represent a good trade-off between the classification accuracy and the reduction rates.

In relation to the prototype-based decision rules, in general, the classification accuracy obtained by the FLD tends to be higher than that of the NQC, both higher than the accuracy of the 1-NN rule, independently of the considered condensing algorithms. This is striking as the prototype sets are often optimised to guarantee that the 1-NN rule performs well. Our explanation is that the FLD and the NQC, although based on the condensed sets, still make use of the entire TS for determining the decision boundary. The 1-NN rule, when applied as a nearest prototype rule, discards other training objects.

What is important, is the fact that for the evaluation of new objects the computational complexity of the FLD is $O(Jr)$. This is similar to the computational complexity of the 1-NN rule, $O(r)$, provided that $J$, the number of classes, is small. For a large number of classes, the computational cost of the FLD increases. The FLD may, therefore, be an
alternative to the 1-NN rule for the prototype-based classification in normalised feature vector spaces. The NQC is much more computationally heavy, so it can only be advantageous for small condensed sets and a small number of classes. In fact, the NQC was used here, to show that a more complex classifier than a linear one is not necessarily yielding a better performance in dissimilarity spaces resulting from normalised vectorial data. The effect of feature normalisation plays a role as otherwise the NQC might have been preferred to the FLD. In general, the good performance of the FLD in dissimilarity spaces can be explained by the use of Euclidean distance relying on standardised features (hence approximate normal distributions for the resulting distances) and non-complicated class structures for which this distance measure is discriminative. The later means that the classes do not differ much in the range of their average within-class distances.

Our final conclusion is that the adaptive techniques, the LVQ and the MixtGauss, combined with the FLD, offer the best trade-off between the reduction rate, computational cost and the classification performance in normalised vector spaces for the considered problems.

In perspective, our study opens a new possibility for using linear (or more complex) classifiers in dissimilarity spaces derived from normalised feature vector spaces instead of the 1-NN rule, both defined by the same optimised prototype sets. Since a linear function in such a dissimilarity space is a non-linear function in the original vector space, the distance measure or its non-linear (sigmoidal, logarithmic) transformation can be a way to incorporate the non-linearity aspects of the data. To our knowledge, these aspects have not been considered among the researchers studying the condensing techniques, yet. Although the FLD was chosen here, other linear functions can be studied, such as a logistic classifier or a hyperplane defined by a linear, sparse or non-sparse, programming procedure. Additionally, a linear (or polynomial) support vector machine (SVM) [32] can be trained in dissimilarity spaces. Note, however, that in such a case the SVM will rely on support vectors which are objects found in a complete dissimilarity space, hence they rely on the distances to all original objects. So, the SVM will not work as a prototype selection. If however, good prototypes are found by other techniques, the linear SVM will determine the optimal large-margin hyperplane in the corresponding dissimilarity space. Future research may focus on comparing a (non-)linear SVM built in the original feature vector space and the SVM in a dissimilarity space defined by a small set of optimised prototypes.

Acknowledgments

This work has been partially supported by grants DPI2001-2956-C02-02 and TIC2003-08496 from the Spanish CICYT and project IST-2001-37306 from the European Union, as well as by the Dutch Organisation for Scientific Research (NWO).

References

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