

Heterogeneous distance functions for prototype rules: influence of parameters on probability estimation.

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Abstract: An interesting and little explored way to understand data is based on prototype rules (P-rules). The goal of this approach is to find optimal similarity (or distance) functions and position of prototypes to which unknown vectors are compared. In real applications similarity functions frequently involve different types of attributes, such as continuous, discrete, binary or nominal. Heterogeneous distance functions that may handle such diverse information are usually based on probability distance measure, such as the Value Difference Metrics (VDM). For continuous attributes calculation of probabilities requires estimations of probability density functions. This process requires careful selection of several parameters that may have important impact on the overall classification of accuracy.

In this paper, various heterogeneous distance function based on VDM measure are presented, among them some new heterogeneous distance functions based on different types of probability estimation. Results of many numerical experiments with such distance functions are presented on artificial and real datasets, and quite simple P-rules for several heterogeneous databases extracted.

Keywords: Prototype rules, probability estimation, heterogeneous distance functions, similarity-based methods, classification, data mining.

1 Introduction

Many important problems in artificial intelligence may be reduced to classification problems. Despite the problem, this is still a very active research area. Many different approaches to classification have been proposed, including such popular methods as artificial neural networks or support vector machines. Unfortunately their possible applications are limited, because they usually act as black boxes, and it is impossible to understand their decisions in logical terms

(however, it is possible to visualize them [1]). For some inputs their decisions may be unpredictable, leading to disastrous consequences. This constitutes the reason why they may be dangerous to use in decision support systems that require transparency of decisions. If some understanding of data is demanded, machine learning algorithms for logical rule extraction are used [2]. The challenge is to generate a set (or multiple sets) of rules that will be reliable, accurate and easy to understand by humans. Although the need for rule-based descriptions is generally acknowledged, many methods create too many rules with too complex conditions, which, in effect, results in incomprehensible descriptions of data. In such a case it may be better to use reliable pattern recognition classifiers rather than rules.

Statistical approaches based on the “divide-and-conquer” idea lead to univariate decision trees that generate crisp logic rules operating on each attribute separately. The most popular examples are Quinlan’s C4.5, Breiman’s CART [3] or SSV tree algorithms [4]. Expressive power of crisp rules (C-rules) is rather limited, therefore fuzzy rules (F-rules), generated by neurofuzzy systems [5] are frequently used, although they may sometimes generate rather complex description of the data that is hard to understand, even though a simple crisp set of rules exists [2]. An alternative is offered by recently introduced prototype-based rules (P-rules) [6, 7]. The F-rules and P-rules may be transformed into each other and allow to express more interesting concepts than crisp logic rules. Experiments showed that both approaches are usually capable of generating highly accurate, yet small and understandable sets of rules.

To specify F-rules the shape of membership functions has to be defined, and parameters determining rule properties have to be estimated from the data. For P-rules the type of distance measure has to be defined. The usual choice is the Euclidean distance function or more generally the Minkovsky’s family of distance functions. However, in practical applications it is not always the best solution. In real world, most datasets have mixed types of attributes, with some real-valued, some discrete, and some symbolic or nominal ones. For such data, Euclidian distance functions are not directly applicable. In case of symbolic features results will depend on the method of conversion from nominal to numeric values. This problem also plays a role in fuzzy rules, where it is sometimes not clear what type of a specific membership function is appropriate.

Mixed types of attributes may be used in heterogeneous distance functions that use different types of measures for different types of attributes, combining information contained in their differences. This type of functions are usually based on probability distance measures, such as the Value Difference Metric (VDM) [8], adopted for continuous attributes by estimating probability density function for real feature values. The process of estimation requires the selection of several parameters that may have an important influence on overall classification accuracy. This is the subject of this paper.

Section 2 describes relations between F-rules and P-rules, and advantages which may be derived from this relation. In section 3 different heterogeneous distance function based on VDM measure are presented. Section 4 presents some new heterogeneous distance functions based on different types of probability estimation. Numerical experiments on artificial and real data are presented in section 5, and, in section 6, the summary of results is given, and some conclusions are drawn.

2 F-rules versus P-rules

Classical crisp logical rules are quite easy to understand, seem to be natural to most people, are easy to apply, and, therefore, are in wide use in decision support and similar applications. However, if the goal is to understand real-world data collected from some experiments crisp rules may often fail, because a large number of these rules with many conditions may be needed, making it impossible to understand the structure of the data. F-rules and P-rules are much more flexible and a smaller number of such rules may be sufficient. Thus, also more robust and easier to understand.

The process of learning F-rules starts with selecting the shape of membership functions (MF), their initial position separately for each feature as well as selecting appropriate fuzzy operators like T-norms, aggregation operators and inference scheme [5]. In the second step of the learning process algorithms tune the spread and position of each membership function and try to select appropriate combination of these functions to extract fuzzy if-then rules. Such methods are often based on neural adaptation algorithms, and therefore are called neuro-fuzzy systems.

In P-rules the goal is to optimize the position of prototypes to which unknown vectors will be compared using previously chosen distance function or similarity measure. Two different types of P-rules exist. First, the nearest neighbour rules (NNR), where the distance is calculated between unknown case and all the prototypes, and the prototype that is most similar is used in the condition part of the rule, claiming that the output class is the same as the class of the nearest prototype:

$$\text{IF } P' = \arg \min_{a=1:L} D(X, P_a) \text{ THEN } C(X) = C(P')$$

where \mathbf{X} is the input vector, \mathbf{P}_a is one of the L prototypes, and $C(\mathbf{P})$ is a function returning the label of the vector \mathbf{P} . These rules are discriminative, and for two prototypes from different classes define a decision hyperplane between them.

P-rules of the second type are threshold rules (TR) where each prototype has associated threshold value defining subspace of activation and all vectors that fall into this subspace have output label that is the same as this prototype label.

$$\text{IF } D(X, P) < \text{Tr} \text{ THEN } C(X) = C(P)$$

where Tr is threshold value. These rules provide coverings of parts of the feature space.

F-rules, and more precisely their MF, have four major interpretations [8]. One of the most popular and natural interpretations tries to explain MF as a degree to which elements of universe X are similar to or typical of a fuzzy set F defined by its MF. From this perspective, F-rules seem to be a special case of similarity-based learning (SBL) [10]. This observation leads to new perspectives in both fields: SBL and Fuzzy Modelling. New distance functions may be derived from membership functions, and vice versa [6,7]. The simplest example is transformation between additive distance functions, which is equivalent to a product of MF using exponential transformation function:

$$D(\mathbf{x}, \mathbf{y})^2 = \sum_{i=1}^m w_i (x_i - y_i)^2$$

$$F_\mu = \exp(D(\mathbf{x}, \mathbf{y})^2) = \exp\left(\sum_{i=1}^m w_i (x_i - y_i)^2\right) = \prod_{i=1}^m \exp(w_i (x_i - y_i)^2)$$

$$F_\mu = \prod_{i=1}^m \mu_i(x_i); \quad \mu_i(x_i) = \exp(w_i (x_i - y_i)^2)$$

The main weakness of F-rules is the difficulty in their application to heterogeneous datasets. Theoretically, fuzzy sets can also be defined for arbitrary features, however most of the neurofuzzy systems (ex. NEFCLASS, ANFIS) do not support symbolic or non ordered attributes, and are defined only for real input values [5]. The problem with automatic construction of MFs for nominal attributes may be solved using the SBL approach. Probability-based distance functions, such as VDM metrics, may be defined for any type of features, and they may be combined with real-valued features in heterogeneous distance functions (HDF) [11]. They are described in the next two sections.

3 Heterogeneous Distance Functions

In most similarity based systems, such as the nearest neighbour [3], Radial Basis Function networks, or self-organizing maps [12], Minkovsky's distance function are used, sometimes in rotated coordinate systems, or, for example the Mahalanobis distance function. Unfortunately, this type of distance functions does not support symbolic and nominal features that are often found in real applications. On the other hand, the Value Difference Metrics (VDM) and similar metrics [8] give very good results for symbolic attributes, but using it directly with continuous attributes is impossible. To construct prototype-based rules for datasets with

different types of attributes both types of similarity functions should be combined in a heterogeneous distance function [11].

VDM distance measure is based on calculation of differences between posterior probabilities:

$$VDM(\mathbf{X}, \mathbf{Y}) = \sum_{a=1}^m vdm(x_a, y_a) \quad (1)$$

$$vdm(x_a, y_a)^2 = \sum_{i=1}^n (p(C_i | x_a) - p(C_i | y_a))^2 \quad (2)$$

where probabilities are estimated by frequencies:

$$p(C_i | x_a) = \frac{Nx_{ai}}{Nx_a} \quad (3)$$

\mathbf{X} and \mathbf{Y} are input vectors, Nx_a is a number of instances in a training set with value of x_a for the attribute a , Nx_{ai} is the same as N_a but for the class C_i , n is the number of classes and m is the number of attributes. P-rules use heterogeneous distance functions (HDF) for features of mixed types. One of the simplest ways leading to the HDF is the combination of the Euclidean and VDM metrics, called the Heterogeneous Value Difference Metric (HVDM) [10]:

$$HVDM(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{a=1}^m d_a^2(x_a, y_a)} \quad (4)$$

where

$$d_a(x, y) = \begin{cases} 1, & \text{x or y are unknown} \\ n_vdm_a(x, y) & \text{a is discrete or nominal} \\ n_dif_a(x, y) & \text{a is continuous} \end{cases} \quad (5)$$

For the nominal data, $d_a(x, y)$ assumes one of the forms:

N1:

$$n_vdm_a(x, y) = \sum_{i=1}^n \left| \frac{Nx_{ai}}{Nx_a} - \frac{Ny_{ai}}{Ny_a} \right|$$

N2:

$$n_vdm_a(x, y) = \sqrt{\sum_{i=1}^n \left| \frac{Nx_{ai}}{Nx_a} - \frac{Ny_{ai}}{Ny_a} \right|^2} \quad (6)$$

N3:

$$n_vdm_a(x, y) = \sqrt{n \cdot \sum_{i=1}^n \left| \frac{Nx_{ai}}{Nx_a} - \frac{Ny_{ai}}{Ny_a} \right|^2}$$

and for continuous data

$$n_vdm_a(x, y) = \frac{|x - y|}{4\sigma_a} \quad (7)$$

where σ is the standard deviation for the attribute a . The Euclidean distance used by HVDM for continuous features is normalized by standard deviation of the attribute to reduce the influence of the outliers.

Three different forms of VDM distance with different normalization technique are used, and the decision which one should be chosen depends on a designer of the system. The main problem using HVDM is normalization, because it is very difficult to balance different terms in the overall distance metric. This problem does not occur for the Value Difference Metric where posterior probabilities are estimated for both discrete and continuous features. However, in such a case the estimation of probability density for continuous features is a big problem. Martinez and Willson [10] also described Discretized Value Difference Metric (DVDM) and Interpolated Value Difference Metric (IVDM).

DVDM is based on discretization process, and for continuous attributes a simple constant width discretization method is used. DVDM is defined by the equation:

$$DVDM(\mathbf{x}, \mathbf{y})^2 = \sum_{a=1}^m vdm_a(disc_a(x_a), disc_a(y_a))^2 \quad (8)$$

Where $disc$ is a discretization function defined as:

$$disc_a(x_a) = \begin{cases} \left\lfloor \frac{x - \min_a}{w_a} \right\rfloor + 1 & \text{if } x \text{ is continuous} \\ x & \text{if } x \text{ is discrete} \end{cases} \quad (9)$$

\min_a is the minimum of attribute a and w_a is a parameter describing the number of discretization bins. However, the upper part of equation (9) can be replaced by a different form of discretization algorithm.

IVDM is very similar to DVDM, but to improve the accuracy of posterior probability estimates a simple linear interpolation is used. IVDM is defined by:

$$IVDM(\mathbf{x}, \mathbf{y}) = \sum_{a=1}^m indm_a(x_a, y_a) \quad (10)$$

$$indm_a(x_a, y_a) = \begin{cases} vdm_a(x_a, y_a) & \text{a is discrete} \\ \left(\sum_{i=1}^n p_{ai}(x) - p_{ai}(y) \right)^2 & \text{a is continuous} \end{cases} \quad (11)$$

where

$$p_{ai}(x) = p_{ai} + \frac{x - mid_{au}}{mid_{a,u+1} - mid_{a,u}} \cdot (p_{ai,u+1} - p_{ai}) \quad (12)$$

Here p_{aiu} and $p_{ai,u+1}$ are posterior probabilities calculated in the middle of the discretized range u and $u+1$, $u = \text{disc}(x)$ and mid_{au} and $mid_{a,u+1}$ are middles of discretized ranges u and next $u+1$, for which actual x_a fulfil inequality.

4 New Heterogeneous Distance Functions

The main problem in the application of VDM distance measure to continuous attributes is to obtain appropriate shape of posterior probabilities. For discrete or symbolic features they can easily be computed using frequencies, Eq. (3), but for continuous attributes it will not work. Two simple techniques were presented in the previous section, but a better algorithm used for determining posterior probabilities may lead to a better overall results. These new methods are based on equation (11), but with a different density estimation technique.

4.1 Gaussian Value Difference Metric

Kernel smoothing techniques, for example Gaussian smoothing kernels, allow to calculate the posterior probability as:

$$p(C_i | x_a) = \left(\sum_{j=1}^{M_i} \exp \left[- \left(\frac{x_{aj}}{\sigma} \right)^2 \right] \right) \cdot \text{norm} \quad (13)$$

where M_i is the number of all vectors from the same class C_i , σ is the width of Gaussian functions, and norm is the normalization factor calculated by:

$$\text{norm} = 1 / \sum_{k=1}^n \left(\sum_{j=1}^{M_i} \exp \left[- \left(\frac{x_{aj}}{\sigma} \right)^2 \right] \right) \quad (14)$$

4.2 Local Value Difference Metric (LVDM)

Very simple and very fast technique for estimating probability is based on the Local Value Difference Metric (LVDM). This method uses local calculation of probability density surrounding the query data point. In this method, probability is calculated by the equation (3), but the value of $N_{x_{ai}}$ is the number of points in class C_i in the range limited to $\left[x_a - \frac{\text{width}_a}{2}, x_a + \frac{\text{width}_a}{2} \right]$, and N_{x_a} is similarly calculated in this range for all classes. Width_a is a parameter defining a range of widths for attribute a .

4.3 Parzen Value Difference Metric (PVDM)

Another solution for density estimation is based on the Parzen Window technique [3] where a rectangle window is moved by the step through the whole

range of attribute a , and probability is calculated as a mean value of all window probabilities where x occurs:

$$p(C_i | x_a) = \frac{1}{Z} \sum_{z=b+1}^{b+Z} \frac{N_{iz}(x_a)}{N_z(x_a)} \quad (15)$$

where Z is number of windows, $Z = \frac{width_a}{step_a}$, b is the index of first window where x

occurs, $N_{iz}(x_a)$ is the number of data points in z -th window that belong to class C_i , $N_z(x_a)$ is summed over all classes, $width_a$ is the window width for attribute a , and $step_a$ is the size of the window movement.

5 Numerical Experiments

Experiments were performed on artificial and real data. The artificial data were generated to check the quality of probability estimations, and the influence of the parameters used on the probability estimation accuracy. Two artificial datasets were generated for this purpose. First dataset had two dimensions, 3 classes, with vectors for each class generated from a normal distribution. The second dataset also had two dimensions and 3 classes, but data vectors were generated using uniform distribution. In both datasets classes were partially overlapping.

In the second set of experiments P-rules were generated using probabilistic distance functions for several datasets taken from the UCI repository of machine learning datasets [13]. For these experiments different datasets were selected with different types of attributes: continuous, discrete, symbolic and nominal.

All tasks were carried out with SBPS software system especially developed for that purpose. SBPS is a similarity based rule generating system that allows for defining different types of distance functions for different attributes and combining the results obtained with each feature into a final value. SBPS system includes several prototype selection and optimization algorithms, which are used to simplify and improve initial rules. To compare the results obtained in different experiments only Fuzzy C-means algorithm for prototype selection and LVQ algorithm for their optimization have been used [12].

5.1 Artificial datasets

Artificial datasets were created to verify the quality of five methods for probability estimation, compare them with a heterogeneous distance function, and evaluate the influence of parameters of these methods on the final classification results. For the first artificial dataset with normal distribution of samples in each class optimal border shape can be obtained using Euclidean distance function. These results determine a basis to judge and compare quality of probability estimation and classification for other functions. In this test only one prototype per class was

generated. To reduce the influence of randomness and verify generalization 10-fold crossvalidation test was performed. Results presented in Tab. 1 show balanced accuracy for each method.

Table 1. Balanced accuracy for different methods of probability estimation obtained on artificial datasets

		HVDM	GVDM			LVDM				IVDM		DVDM	
			sig 0.2	sig 0.5	sig 0.7	width 0.2	width 0.4	width 0.6	width 0.8	CW 10	CW 5	CW 10	CW 5
Dataset 1	Bal. Acc	96.83	95.67	96.80	96.17	95.00	95.33	95.50	95.33	95.17	94.33	96.50	90.50
Dataset 2	Bal. Acc	90.50	88.33	90.67	90.33	86.00	88.17	88.33	89.00	86.83	87.50	85.17	81.33
		PVDM											
		Step 0.1				Step 0.01				Step 0.05			
		W 0.2	W 0.4	W 0.6	W 0.7	W 0.2	W 0.4	W 0.6	W 0.7	W 0.2	W 0.4	W 0.6	W 0.7
Dataset 1	Bal. Acc	94.67	94.83	95.83	96.17	95.00	95.50	96.00	96.50	94.67	94.00	96.00	96.17

5.2 Real datasets

The 6 types of VDM distance functions have also been tested on real datasets to verify theoretical considerations. Several datasets with different types of attributes were selected from the UCI repository: Flag, Glass, Iris, Lancet and the Pima Indians. Since the aim was to obtain maximum balanced accuracy for all these distance measures, we have used the algorithm for constructive rule generation to maximize classifier abilities.

The constructive algorithm for generation of P-rules does not favour any distance function because it adds a new prototype to the class with lowest accuracy, maximizing overall balanced accuracy calculated as a mean value of individual accuracies. In all cases, the algorithm was stopped after 10 iterations, generating at most 10 prototypes per class.

Table 2. Balanced accuracy for different methods of probability estimation obtained on real datasets

HVDM	flag Bal. Acc	glass Bal. Acc	iris Bal. Acc	lancet Bal. Acc	pima Bal. Acc
	18,958	37,772	96,000	90,228	73,740
GVDM					
sig 0.2	23,229	48,948	96,000	89,994	71,815
sig 0.5	30,208	55,367	96,667	89,777	71,401
sig 0.7	28,438	46,865	96,667	89,777	71,386
mean	27,292	50,394	96,444	89,849	71,534
std	3,628	4,431	0,385	0,126	0,244
LVDM					
width 0.2	25,625	47,778	96,000	90,103	72,886
width 0.4	27,708	44,147	96,667	89,994	72,049
width 0.6	26,563	48,978	95,333	89,994	71,490
width 0.7	26,875	42,054	94,000	89,777	71,676
mean	26,693	45,739	95,500	89,967	72,025
std	0,861	3,202	1,139	0,137	0,619
PVDM					
W0.2 St0.1	30,104	39,722	96,667	90,103	71,613
W0.4 St0.1	26,563	42,639	96,667	89,994	71,504
W0.6 St0.1	24,375	49,702	95,333	89,777	70,531
W0.7 St0.1	27,396	49,206	96,667	89,876	71,034
W0.2 St0.01	29,479	46,359	96,000	90,005	71,820
W0.4 St0.01	25,625	45,694	96,000	89,994	71,468
W0.6 St0.01	24,375	58,046	96,667	89,777	71,234
W0.7 St0.01	27,083	48,075	96,667	89,777	71,041
W0.2 St0.05	28,542	46,319	96,000	90,103	71,386
W0.4 St0.05	26,250	44,345	96,000	89,994	71,482
W0.6 St0.05	24,375	56,141	96,000	89,777	70,970
W0.7 St0.05	27,813	56,379	96,667	89,777	71,555
mean	26,832	48,552	96,278	89,913	71,303
std	1,953	5,717	0,446	0,133	0,355
IVDM					
CW 10	26,563	46,984	96,000	90,225	70,818
CW 5	26,042	48,651	96,667	90,117	72,375
mean	26,302	47,817	96,333	90,171	71,597
std	0,368	1,179	0,471	0,077	1,101
DVDM					
CW 10	26,979	43,810	97,333	90,325	71,081
CW 5	27,083	50,635	94,667	90,330	70,142
mean	27,031	47,222	96,000	90,327	70,612
std	0,074	4,826	1,886	0,003	0,664

Because of the normalization problem of different distance functions, all continuous features in all datasets were standardized and then normalized to the interval [0,1]. The highest balanced accuracy for each combination of parameters for all datasets is presented in Table 2.

6 Discussion of results and conclusions

The “no free lunch” theorem [3] says that no single algorithm for data analysis may always be the winner, and the results presented in Tab. 2 certainly confirm it. For artificial data the GVDM algorithm seems to be better than other estimation methods. It could be expected that this algorithm should give a very good results for this type of artificial data, with high density of points, generating the smoothest estimated probability distributions, but selection of appropriate parameters has significant influence on the estimations.

Results on real datasets show that choosing correct algorithm parameters is now very important and selection of single best distance function is impossible. In Table 2 the highest accuracies, marked in bold, appear for different methods for each dataset. The GVDM distance does not work so well now, sometimes giving large variance of results for different parameters of probability estimation algorithms. These results, unfortunately, do not lead to any definite conclusion about what type of distance should be used or which values of parameters are the best. If some values of estimation parameters are wrongly chosen, contours of probability distribution may be very jagged and important information about data may be lost.

Some general conclusions about appropriate values of estimation parameters may be reached. For LVDM distance it is impossible to select accurate window size, for example, for the Flag dataset the most appropriate value is 0.4, but on the Glass dataset for the same value almost the worst results have been obtained; still the standard deviation of the accuracy for LVDM is rather small for all datasets, making this method rather insensitive to the choice of its parameters.

Much better but less stable results were obtained with GVDM algorithm. Although for all datasets $\sigma=0.5$ leads to the best or nearly the best results, the variance of these results is larger. DVDM and IVDM methods were tested only with two significantly different parameter values, but the differences in accuracy is rather small for these methods. The Parzen window PVDM algorithm tends to prefer small step sizes, with the best results achieved with step 0.05 and 0.01, while the step size of 0.1 led to the worst results; also a wider window is preferred, about 0.6-0.7.

The comparison between different methods is not so clear, calculations performed on some datasets show that even the simplest DVDM measure may sometimes give good results. This situation occurs when a gap between different classes is very small, and the more advanced techniques that use smoothing usually lead to an increased number of errors; it is especially important for datasets with small number of training vectors.

An interesting extension of the work described here may be done by replacing VDM metric function with another probability distance metrics, such as the Minimum Risk Metric (MRM) or Short and Fukunga metric (SFM) [8]. Also other kernel smoothing techniques should be analyzed and compared. A significant influence of more advanced discretization algorithms may be expected. These

methods will be analyzed in the near future. The final goal is to create the simplest and most accurate P-rules for any kind of data.

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