Symbolic Distance Measurements Based on Characteristic Subspaces

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Abstract. We introduce the *subspace difference metric*, a novel heterogeneous distance metric for calculating distances between points with both continuous and (unordered) categorical attributes. Our approach is based on the computation and comparison of *characteristic subspaces* (i.e. contexts) for each of the symbols and can be viewed as a generalization of the well-known *value difference metric*.

Subsequently, as one possible extension, we propose a linearization of the computed symbolic distances by *multidimensional scaling*, thereby mapping a set of symbols onto the interval $[0, 1]$. Thus, even algorithms, which have originally been designed for usage with continuous attributes (e.g. clustering algorithms like k-means), may be applied to datasets containing discrete attributes, without having to adapt the algorithm itself.

Finally, we evaluate the proposed metric and the linearization in quantitative and qualitative settings and exemplify the applicability in clustering domains.

1 Introduction and Motivation

Many inductive algorithms in machine learning and data mining make strict assumptions on the attribute types of the database. On the one hand, algorithms for dealing with continuous data may naturally utilise nearness measurements and exploit the metric properties of the instance space. On the other hand, however, restricting a knowledge structure to categorical data allows for more “exact” induction methods (like association rule or functional dependency mining), because, intuitively, categorical data does not contain that kind of inherent “fuzziness” which continuous data usually exhibits.

Many learning algorithms, most notably instance based techniques, neural networks and some of the most widely used clustering methods, necessitate all attribute types to be continuous – in these cases categorical or nominal data or missing values can often not be handled appropriately. To overcome these difficulties, in the context of classification learning, the *value difference metric* (VDM, refer to [SW86] or [CS93]) or one of its generalizations [WM97] has been used to good effect. Furthermore some interesting approaches for clustering heterogeneous data (i.e. datasets with mixed continuous and categorical attributes) have been published in the recent years.

Some of these novel approaches can be regarded as self-contained methods for clustering: E.g., [GKR00] and [ZFCH00] describe iterative clustering approaches based on dynamical systems, [SCC00] use a generalized notion of entropy, [GRS00] propose a concept of links to measure similarity and [GGR99] introduce a summarization-based algorithm. Additionally, extensions for some well-known clustering algorithms have been developed: E.g., [NH98] describe incremental and sparse variants of the EM algorithm and [GRB99] develop a discrete KMeans algorithm.

Whereas the problem of transforming continuous attributes to discrete types for the application of symbolic algorithms is well-known and usually termed *discretization*¹, none of the aforementioned methods solves the inverse problem: transforming discrete symbols to ordered (continuous or nominal) types. They either represent complete self-contained clustering procedures with little or no affinity to any continuous clustering scheme or require a rewriting of the distance metric used by the clusterer.

In this paper we propose the *heterogeneous subspace difference metric* (HSDM), a novel heterogeneous distance metric for computing distances between points with both continuous and categorical attributes. The basic idea is the computation and comparison of *characteristic subspaces* for each of the symbols, thus, the HSDM can be viewed as a generalization of the HVDM (*heterogeneous value difference metric*).

Furthermore, for usage as a pre-processing step, we propose a linearized extension of the SDM component, the *linearized subspace difference metric* (lSDM), which induces a strict ordering of the involved symbols. For this task we make use of *multidimensional scaling* (MDS) to map a set of symbols onto a one-dimensional scale, given high-dimensional distance measurements calculated by the SDM. Thus, even algorithms, which have originally been designed for usage with continuous attributes, may be applied to datasets containing discrete attributes, without having to adapt the algorithm itself.

2 Categorical Metrics

As [GGR99] note, distance functions on categorical attributes are not naturally defined, because it is difficult to reason that, e.g., “one color is ‘like’ or ‘unlike’ another color in a way similar to real numbers.” This is due to the fact that (unordered) categorical attributes typically do not contain any information other than the symbols themselves. Whereas with continuous numbers various calculations and pairwise comparisons can be performed, usually all we can say about two colors, is whether they are equal or not.

¹ Some induction algorithms can be viewed as being able to discretize “on the fly” (e.g. C4.5), however also several methods for automatic pre-discretization have appeared in print: [DKS95] give an excellent overview, while [Lud00] present an unsupervised multivariate approach.

2.1 Overlap and VDM

This, then, is also the most widely used (e.g. [AKA91]) method for comparing two symbols: For calculating the distance between two instances with mixed continuous and categorical values, the following *heterogeneous euclidean overlap metric* (HEOM, refer to [WM97]) is used:

$$HEOM(\mathbf{x}, \mathbf{y}) = \sqrt{\sum_{i=1}^m d_i(x_i, y_i)^2}$$

Here, $\mathbf{x}$ and $\mathbf{y}$ are instance vectors, m is the number of attributes and d_i is the following function:

$$d_i(x, y) = \begin{cases} 1 & \text{if } x \text{ or } y \text{ is missing} \\ \text{overlap}(x, y) & \text{if attribute } A_i \text{ is categorical} \\ \frac{|x-y|}{\text{range}_i} & \text{otherwise} \end{cases}$$

The following simple *overlap function* is used:

$$\text{overlap}(x, y) = \begin{cases} 0 & \text{if } x \neq y \\ 1 & \text{otherwise} \end{cases}$$

Clearly, the HEOM is overly simplistic in handling categorical attributes and although it may be appropriate in some cases, its use can lead to poor performance [CS93].

A more sophisticated alternative, the *value difference metric* (VDM), introduced by [SW86], in most cases provides a better distance measurement for categorical attributes: Basically, it consists of considering two symbols to be similar, if they make similar predictions. The following definition is a simplified version without weighting terms [Dom96]:

$$SVDM(x, y) = \sum_{i=1}^c |p(c_i|x) - p(c_i|y)|^q$$

where c is the number of classes, $p(c_i|x)$ is the conditional probability that the output class is c_i given the input value x and q is a constant (usually 1 or 2). This categorical distance function can then be used as a replacement for the overlap function, yielding the *heterogeneous value difference metric* (HVDM, refer to [WM97]).

As [Dom96] note, the SVDM “attenuates [the problem of sensitivity to irrelevant attributes] for symbolic attributes, as long as a large number of examples is available, [...] due to the fact that by definition $p(c_i|x_j)$ will be roughly the same for all values x_j of an irrelevant attribute, leading to zero distance between them.” However, the SVDM is obviously only applicable in cases, where class values are available for all instances (e.g. classification tasks).

2.2 The Subspace Difference Metric (SDM)

In situations, where a class attribute is not readily available (e.g. unsupervised learning), the VDM obviously cannot be used by definition. In such cases one might be tempted to fall back on the simpler *overlap function* to compute heterogeneous distances. With datasets, where the majority of attributes is continuous, this procedure might be appropriate – or at least not too harmful –, but when many or all of the attributes are of categorical type, much information about the distribution of the symbols will be lost thereby.

Rethinking the first paragraph in section 2, we realize that it is not exactly true. Actually, we do have more information about the symbols of a categorical attribute: we know (or can compute) the distribution of each symbol within the instance space, i.e. we know what values in other attributes each symbol co-occurs with. And this is exactly the information that we need to be able to argue that, say, the color **red** is more similar to **orange** than to **blue**.

Intuitively, to be able to argue about the pairwise similarity of two symbols, we have to make the assumption that the symbols do not exactly partition the domain space of another attribute. E.g. to be able to say that **red** is more similar to **orange** than to **blue**, we could argue that there are more instances in the dataset which can be **red** or **orange** than there are instances which can be **red** or **blue**. I.e. the context, in which the color **red** occurs overlaps more with the context of the color **orange** than with that of the color **blue**.

Characteristic Subspaces. The ideal tool for computing the overlaps between such contexts would be *characteristic rules* or the *characteristic subspaces* induced by them. Formally:

Definition 1. Let A_i represent the i -th attribute ($i \in \{1, \dots, m\}$) and V_i be a set of values from the domain of attribute i . A characteristic rule is an implication rule of the form

$$A_i = x \rightarrow A_1 \in V_1 \wedge \dots \wedge A_m \in V_m$$

where the attribute A_i does not occur on the right hand side. A characteristic rule is said to hold with confidence p , formally

$$A_i = x \rightarrow_p A_1 \in V_1 \wedge \dots \wedge A_m \in V_m$$

if, with probability at least p , whenever condition $A_i = x$ holds for an instance, the right hand side holds as well.

A characteristic rule is basically an *association rule*, where the left hand side is restricted to only one condition. V_i is a discrete set of values, if A_i is categorical, and a continuous interval, if A_i is continuous.

Usually characteristic rules are constructed for values of a designated class attribute, we may, however, induce such rules for symbols from any categorical attribute. Thereby we obtain information about the context in which a certain symbol occurs – the subspaces induced by these rules will in the following be

called *characteristic subspaces*. Intuitively, a *characteristic subspace* gives an extensional description of a symbol and by comparing these spaces we could argue about the similarity of the symbols.

Projected Characteristic Subspaces. Unfortunately, computing such *characteristic subspaces* with high *confidences* would necessitate running a characteristic rule induction algorithm for each single symbol, which is obviously computationally infeasible. For rules with high confidence it would, e.g., not suffice to compute the projections of a symbol onto each of the other attributes and combine them, because the cartesian product of two or more highly probable regions in different attributes need not necessarily be highly probable as well, formally:

$$A_i = x \rightarrow_p (A_j \in V_j), A_i = x \rightarrow_p (A_k \in V_k) \not\Rightarrow A_i = x \rightarrow_p (A_j \in V_j \wedge A_k \in V_k)$$

However, in our case, we may relax the requirements, in that we actually need not construct full *characteristic subspaces*. For the comparison of two symbols it does suffice to compare the projections onto each of the other attributes. We call the resulting spaces *projected characteristic subspaces* (*pc-subspaces*).

Definition 2. With D_i representing the domain of attribute A_i , let the discrete domain $\overline{D}_i$ be defined as follows:

$$\overline{D}_i = \begin{cases} D_i & \text{if attribute } A_i \text{ is categorical} \\ \{1, \dots, d\} & \text{if attribute } A_i \text{ is continuous, for } d \in \mathbb{N} \end{cases}$$

To construct the *discrete domains* of the attributes, we have to discretize the continuous attributes by some simple unsupervised discretization method. Preferably we should use *equal-width* discretization for this task, because this method visualizes the distribution of the values within the interval (in the experiments we chose $d = 6$ as standard setting).

Definition 3. Let p_j be the discrete probability density of the values from the discrete domain $\overline{D}_j$ of attribute j and let $p_{j,A_i=x}$ be this discrete probability density under the condition $A_i = x$ (i.e. $p_{j,A_i=x}(y) = p_j(y|A_i = x)$). Then the probabilistic projected characteristic subspace (*ppc-subspace*) of the symbol x in attribute A_i is defined as the collection of all densities $p_{j,A_i=x}$ for $j \neq i$.

Definition 4. With m being the number of attributes, x and y symbols from a categorical attribute A_i and $q \in \mathbb{N}$, the subspace difference metric (*SDM*) is defined as follows:

$$SDM_i(x, y) = \sum_{\substack{j=1 \\ j \neq i}}^m \sum_{v \in \overline{D}_j} |p_{j,A_i=x}(v) - p_{j,A_i=y}(v)|^q$$

For convenience and ease of computation, the *ppc-subspace* of a symbol can be written as a matrix of dimensions $m \times s$, with m being the number of attributes and $s := \max\{|\overline{D}_1|, \dots, |\overline{D}_m|\}$. The positions in this matrix are the respective conditional probabilities; columns having less than s symbols are filled with zeros up to s elements. That way, the calculation of a symbolic distance can be seen as a matrix operation.

Finally, plugging the SDM into the heterogeneous metric, where previously the (S)VDM or the overlap function was used, yields the HSDM:

Definition 5. *With m being the number of attributes and $q \in \mathbb{N}$ the heterogeneous subspace difference metric (HSDM) of two instances $\mathbf{x}$ and $\mathbf{y}$ is defined as follows:*

$$HSDM(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^m d_i(x_i, y_i)^q$$

with the distance function d_i defined heterogeneously as follows:

$$d_i(x, y) = \begin{cases} 1 & \text{if } x \text{ or } y \text{ is missing} \\ SDM_i(x, y) & \text{if attribute } A_i \text{ is categorical} \\ \frac{|x-y|}{range_i} & \text{otherwise} \end{cases}$$

Complexity. Due to the fact that the *ppc-subspace* of a symbol can be written as a matrix of dimensions $m \times s$ (section 2.2) the comparison of two symbols is linear in the number of attributes m and in the maximum number of unique symbols s in any categorical attribute. Thus, the computation of a heterogeneous distance between two instances is, in the worst case, $O(m^2s)$. Unfortunately, however, the explicit pre-computation of the *ppc-matrices* would take time $O(m^2n^2)$ (n being the number of instances), yielding $O(n^2)$ complexity for the computation of a dissimilarity matrix as well.

By means of a hashtable, however, many of the computations can be simplified. If, e.g., a complete dissimilarity matrix is to be computed, the *ppc-subspaces* of all symbols can be pre-computed by scanning through all instances and recording each co-occurrence of two symbols x and y in two attributes a_1 and a_2 . That way, the *ppc-subspace* of a symbol is only implicitly represented by all associations (along with their counts) for the according symbol stored in the hashtable. This pre-computation step basically consists of linearly scanning the database and thus can be realized in time $O(m^2n)$.

3 Linearization by Multidimensional Scaling

One possibility for modularly implementing the SDM in a learning algorithm is the HSDM as defined above. However, this necessitates (at least partly) a rewriting of the involved algorithm. Unfortunately, this is not always possible. Also, it may prove advantageous for subsequent quantitative data mining techniques to have available nearness information between the symbolic values.

A transformation of the categorical attributes to continuous types in a pre-processing step could thus be a possible solution. However, we have to be aware of the fact that this task can not always be performed well and that in some cases the simple overlap metric might indeed be more appropriate.

We now extend the SDM to a linearized version, the *linearized subspace difference metric* (ISDM). We accomplish this by applying *multidimensional scaling* (MDS) methods to the distance measurements induced by the SDM.

MDS is typically used for computing representative data points for high-dimensional data (which should, e.g., be visualized) or proximity data (sometimes even incomplete) in a suitable low-dimensional space, such that the distances between the projected data points match the original distance values as faithfully as possible. The basic idea consists of minimizing a cost function, usually *stress*, *raw stress*, *strain* or something similar. The original algorithm for minimizing stress can be found in [Kru64], Sammon mapping, also one of the oldest approaches, can be found in [Sam69]. [dLJ77] describe the widely used majorization method for MDS and [KB97] present an application of deterministic annealing to the problem.

In our case the task can be defined as projecting data points of $m \times s$ dimensions (see section 2.2) onto a continuous scale, i.e. one dimension. For this projection we applied a simple gradient descent approach, minimizing *raw stress*.

The usual problem of finding good initial configurations applies here as well: Applying a strict gradient descent algorithm to a one-dimensional configuration can only move the points around a bit, but cannot change their relative order. However, because the target space is only one-dimensional, we have available a few canonical configurations, which should work reasonably well as starting points:

For a categorical attribute A_i we construct $|\overline{D}_i|$ different initial configurations by using one of the symbols x_j as the point of origin and placing the other symbols at positions which conform to their distances from x_j . We then run the gradient descent algorithm on each of the $|\overline{D}_i|$ configurations and accept the final configuration with the lowest *raw stress* as the resulting projection.

4 Experimental Evaluation

4.1 Quantitative Results

In a first set of experiments we exemplify the applicability of our approach in a clustering setting: We chose several datasets with varying characteristics from the UCI Machine Learning Repository and from the Esprit Project StatLog.

Apart from **hayes-roth** and **postoperative (patient)**, all datasets had both continuous and categorical source attributes. As reference clusterings (for the calculation of *recall*) we used the class labels²; in case of the **servo** dataset,

² It is reasonable to assume that the existing class labels correlate with well-defined subspaces within the instance space. There is, however, no theoretical argument corroborating this assumption.

where the target variable is continuous, we chose to pre-discretize the target by equal-width into 6 classes (i.e. clusters).

The synthetic dataset had five attributes: The attributes 1, 3 and 4 were continuous (ranges $[1, 100]$, $[1, 50]$ and $[1, 100]$, respectively), while the attributes 2 and 5 were symbolic: $\{A, B\}$ and $\{w, y, o, r\}$. The following rules held for the class attribute: $(a_2 = A \wedge a_3 \geq 20 \rightarrow class = 1)$, $(a_2 = B \wedge a_3 \leq 15 \rightarrow class = 2)$, $(a_5 = w \rightarrow class = 3)$ and $(else \rightarrow class = 4)$.

As a clusterer we used the k-means implementation *pam* [KR90], which relies on the pre-computation of a dissimilarity matrix before clustering, from the *cluster* package of the freely available and widely used statistics software R. We compared three different methods: In the first two runs we used *daisy*³ and the HSDM⁴, respectively, for the computation of the dissimilarity matrix before applying *pam*. In a third run we used the LSDM to transform the symbols into real numbers and applied *pam* to the continuous dataset.

For each clustering thus generated we computed two different quality measures: On the one hand we used the *silhouette coefficient* from [KR90] as an internal measure. On the other hand we used *recall* (refer to [LW02]) to compare the resulting clustering to the reference clustering. Table 1 shows the results.

Table 1. Comparative clustering results for various datasets. Shown are the *silhouette widths* (“silh”) and *recall* values (tolerance = 0.5) of k-means clusterings. The highest numbers are printed in bold (no significance test applied).

dataset	rows	cols	classes	daisy		hsdm		lsdm	
				silh.	recall	silh.	recall	silh.	recall
postoperative	90	8	3	0.18	0.24	0.18	0.24	0.25	0.24
hayes-roth	132	4	3	0.23	0.00	0.29	0.00	0.33	0.00
servo	167	4	6	0.14	0.12	0.54	0.16	0.38	0.13
synthetic	200	5	4	0.25	0.10	0.40	0.19	0.44	0.05
heart	270	13	2	0.26	0.68	0.24	0.56	0.38	0.40
crx	690	15	2	0.17	0.64	0.18	0.63	0.19	0.66

As can be seen, the HSDM and/or the LSDM in most cases allow for better clusterings: In all cases the *silhouette width* is higher, which is not really surprising, given that the HSDM naturally allows for more accurate distance measurements than the HEOM – a fact that typically has a positive impact on internal quality measures. We have illustrated this consideration by 2-dimensional cluster plots in figure 1.

³ Basically, *daisy* relies on a slightly more sophisticated HEOM to calculate heterogeneous distances by using weighting factors for each attribute. *daisy* is described in detail in [KR90].

⁴ To be able to use the same format for the dissimilarity matrix we implemented the HSDM in pure R-code (no Fortran), which did not use hashtables (refer to section 2.2). Running times are therefore not comparable.

Fig. 1. Cluster plots (mapped to two dimensions) for the synthetic dataset (see text), clustered by k-means (4 centers) in conjunction with the HEOM (daisy) and the HSDM, respectively.

However, in most cases also the *recall* values of SDM-clusterings increase. From these results it is reasonable to assume that a lower clustering quality is largely due to an inappropriate handling of symbolic attributes.

It has to be noted that the HEOM achieved a better *recall* rating in one case and did not do much worse in two others. As mentioned in section 3, this might be due to the fact that in some cases – especially when the symbols have no inherent canonical order – inducing an artificial order instead of using 0-1-equality might actually be detrimental to clustering quality.

4.2 Qualitative Results

In a second experiment we wanted to investigate whether the linearized SDM *lSDM* is able to capture canonical orderings within symbolic attributes, i.e. whether the concept of characteristic subspaces can indeed reflect intuitively obvious orderings and whether these orderings are preserved by scaling the multidimensional information down to only one dimension.

For this test we chose a more complex, but rather small dataset: *Pittsburgh Bridges* (from the UCI repository) is a “design domain” rather than a classification domain, where 5 design descriptions need to be predicted based on 7

specification properties. The dataset has 108 instances with 13 attributes and few missing values. We chose to eliminate the two “identifying” attributes (id and location).

In table 2 we list the orderings induced by applying the LSDM to the discretized version of the dataset. The correct (or intended) orderings of most of the attributes are known, because they have been discretized from numeric values – e.g. the attribute **erected** reflects time epochs from 1818 to 1986. Note that even the attributes **lanes** (which contains 4 nominal values) was treated as discrete in this context.

Table 2. The induced orderings of the symbolic values in the Pittsburgh Bridges domain. Only symbolic attributes with a canonical order are shown, the induced values for the *missing value*-symbol are omitted. Note: Some numbers are presented in reverse order – this, of course, does not affect the resulting metric.

attribute	correct order	induced order
erected	crafts	crafts (2.93)
	emerging	emerging (1.28)
	mature	mature (0.64)
	modern	modern (0.00)
length	short	short (1.83)
	medium	<i>long (1.00)</i>
	long	<i>medium (0.49)</i>
lanes	1	1 (4.22)
	2	2 (2.16)
	4	4 (1.09)
	6	6 (0.00)
span	short	short (0.00)
	medium	medium (1.96)
	long	long (2.72)

As can be seen, linearizing the symbols by the LSDM can re-construct the former orderings in all but one attribute, where the order of *medium* and *long* is inverted. Note that we only list the results for attributes with a known canonical ordering here and omit results for attributes like, e.g., **purpose** (with the values *walk*, *aqueduct*, *rr* and *highway*).

5 Summary and Discussion

We have presented the novel heterogeneous metric HSDM for computing distances between points with categorical or mixed-continuous-categorical attribute values. The approach is based on the concept of (*probabilistic projected*) *characteristic subspaces*, which can also be viewed as a generalization of the well-known *value difference metric*. Additionally, we have introduced the idea of linearizing the high-dimensional distance matrices by *multidimensional scaling*, thereby

yielding the LSDM, a reverse transformation to discretization: encoding symbols by continuous numbers.

We have exemplified in a clustering setting that the HSDM most often yields better results in terms of internal (*silhouette width*) and external (*recall*) clustering quality measures than the widely used HEOM. Finally, in a qualitative setting, we have shown that the LSDM yields good transformations of the involved symbols into real numbers, especially when an obvious canonical order among the symbols exists.

It has to be noted that the transformation does not always produce superior (quantitative or qualitative) results. Especially in cases, when no intuitively obvious order among the symbols can be found, the naive *overlap* function yields slightly better clusterings. This is obviously due to the fact that in such cases, the computation of 0-1-equality is “as good as it gets” and any artificial ordering of the symbols might deteriorate the results. A combination of both approaches in a single metric is one of our future research topics.

Furthermore, the mapping of the high-dimensional subspace data to one continuous dimension is obviously a crucial step in our algorithm. Using a more sophisticated method for MDS might further improve the final transformation and thus is also one of our topics for future research.

Finally, as one reviewer pointed out, it may be expected that the SDM should lend itself well for application in instance based learning tasks (nearest neighbor classification). We have chosen to evaluate the proposed metric in a clustering setting mainly because – unlike the VDM – it was intended to be used without a designated class attribute and will, eventually, be part of a novel clustering algorithm. Evaluating the SDM in IBL settings is a valuable suggestion, which we plan to tackle in the near future.

Acknowledgements

This research is supported by the Austrian *Fonds zur Förderung der Wissenschaftlichen Forschung (FWF)* under grant no. P12645-INF. The Austrian Research Institute for Artificial Intelligence acknowledges basic financial support by the Austrian Federal Ministry for Education, Science, and Culture.

We would like to thank Peter Filzmoser for invaluable discussions and ideas. We would also like to thank the anonymous reviewers for their helpful comments and suggestions.

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