A STUDY ON SIMILARITY MEASURE FUNCTIONS ON ENGINEERING MATERIALS SELECTION

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ABSTRACT

While designing a new type of engineering material one has to search for some existing materials which suits design requirement and then he can try to produce new kind of engineering material. This selection process itself is tedious as he has to select few numbers of materials out of a set of lakhs of materials. Therefore in this paper a model is proposed to select a particular material which suits the user requirement, by using some similarity/distance measuring functionalities. Here thirteen different types of similarity/distance measuring functionalities are examined. Performance Index Measure(PIM) is calculated to verify the relative performance of the selected material with the target material. Then all the results are normalised for the purpose of analysing the results. Hence the proposed model reduces the wastage of time in selection and also avoids the haphazardly selection of the materials in materials design and manufacturing industries.

KEYWORDS

Similarity measure, Performance index, Materials database, Materials selection, Knowledge Discovery

1. Introduction

Processed information is playing a major role in the success of the any industry. Only who can apply the suitable newest information for his product development, is able to survive in the global competition[11]. The latest developments in storage and network technologies have enabled the fast access to information resources and repositories, but there is a lack of facilities to effectively and efficiently search for the required information. To make use of the huge data repositories and information, the field of knowledge extraction from these data repositories will be of major importance in the next decade. Therefore, research on Data Mining and Knowledge discovery has become one of the most important domains of computer science.

Usually the modern Database Management Systems (DBMS) provide fundamental utilities such as searching, retrieving and indexing mechanisms for the management of such relational data [12], which are well-understood and widely applied in many commercial and industrials applications. The traditional DBMS can help the user If the structure of the information to be searched is sufficiently simple and manageable with available data manipulation mechanism of

David Bracewell, et al. (Eds): AIAA 2011,CS & IT 03, pp. 157–168 , 2011. © CS & IT-CSCP 2011 DOI : 10.5121/csit.2011.1314 the DBMS. Requirements of traditional operational data management such as accounting and billing are perfectly met by a commercial DBMS. Therefore, the information infrastructure of most enterprises is based on the latest Relational Database Management Systems (RDBMS). Recently, an increase in the number of applications, processing large amounts of complex and application specific data objects have been observed. Therefore it is the necessity of the day as the latest trends in the industry require to analyse and use the existing huge complex data.

In application domains such as multimedia, medical imaging, Computer Aided Design (AMPTIAC Material EASE 2 CAMS Report), Material Informatics [13], Nanoinformatics [14], Bioinformatics [15], marketing and purchasing assistance, etc., a high efficiency of query processing is crucial due to the immense and even increasing size of current databases. The search in such databases, called non-standard databases, is rarely based on an exact match of objects. Instead, the search is often based on some notion of similarity which is specific to the application. For applications which do not only support transaction oriented search operations, but also provide high-level strategic information or decision making. It is necessary not only to search for objects which are similar to a given query object but rather to analyze the data set as a whole for knowledge discovery. Information which is interesting in the decision making process include common patterns, classifications of data, knowledge about collections of similar objects and exceptional data.

Similar search and Data Mining have become widespread problems of modern database applications. Similar pattern search in databases is a problem of searching extract patterns that matches the target object/Patterns[2]. A general approach is to translate complex object into single or multi dimensional vector by feature transformation function and then to employ search mechanism to retrieve similar object to a given query object. Analysis of similar patterns involves data mining techniques such as association analysis, correlation analysis, classification, cluster analysis, outlier analysis and distance or similarity functions.

This kind of information is commonly referred to as knowledge and the process of deriving such knowledge or higher-level information from a vast amount of transactional data is called data mining or knowledge discovery in databases (KDD)[6]. Because such applications on top of modern databases are also depend on similarity search [16]. The difference to traditional similarity search applications is, however, that these applications do not only raise few, single similarity queries but rather a high number of such queries.

This paper is organized as fallows, A brief introduction to similarity and distance measuring functions are discussed, and a list of 13 such functions are tabled in section 2. Section 3 describes briefly about the engineering material database. Further the performance index measure(PIM) for material selection, Normalized measures and algorithm for similar material selection are elaborated in the section 4. Finally experimental results and conclusion are discusses in section 5 and section 6 respectively

2. SIMILARITY AND DISTANCE FUNCTIONS

From the scientific and mathematical point of view, similarity/distance is defined as a quantitative degree that enumerates the logical separation of two objects represented by a set of measurable attributes/characteristics[4][5]. Measuring similarity or distance between two data points is a core requirement for several data mining and knowledge discovery tasks that involve distance computation. Examples include clustering (k-means), distance-based outlier detection, classification (KNN, SVM), and several other data mining tasks. These algorithms typically treat the similarity computation as an orthogonal step and can make use of any measure. For continuous data sets, the Minkowski Distance is a general method used to compute distance between two multivariate points. In particular, the Minkowski Distance of order 1 (Manhattan) and order 2 (Euclidean) are the two most widely used distance measures for continuous data. The key observation about the above measures is that they are independent of the underlying data set

to which the two points belong. Several data driven measures have also been explored for continuous data. The notion of similarity or distance for categorical data is not as straightforward as for continuous data. The key characteristic of categorical data is that the different values that a categorical attribute takes are not inherently ordered[7]. Thus, it is not possible to directly compare two different categorical values. The simplest way to address similarity between two categorical attributes is to assign a similarity of 1 if the values are identical and a similarity of 0 if the values are not identical. For two multivariate categorical data points, the similarity between them will be directly proportional to the number of attributes in which they match. Various similarity measure functions are enumerated in the literature [16][17] and whose applications are widespread in retrieving information or data from databases.

Properties of similarity / distance measure function are as follows:

 $D(X,Y) \ge 0$ Distance is a non-negative number.

D(X, X) = 0 The distance of an attribute to itself is zero.

D(X,Y) = D(Y,X) the distance is symmetric function

 $D(X,Z)+D(Z,Y) \ge D(X,Y)$ It does obey triangular inequality.

where
$$X_i = \{x_{i,1}, x_{i,2}, x_{i,3}, x_{i,4}, x_{i,5}, \dots, x_{i,n}\}$$
 and $Y_i = \{y_{i,1}, y_{i,2}, y_{i,3}, y_{i,4}, y_{i,5}, \dots, y_{i,n}\}$ are two n dimensional data sets. Any function is said to be a distance metric if it satisfies the properties from 1 to 4, however the similarity function may not satisfy the 4th property.

Some of the distance or similarity function frequently used for information retrieval from the databases are listed below and employed for material selection from the engineering materials database.

Table 1 . Various Similarity/ Distance functions

1.	Euclidean Distance	$D_{Eud}(X,Y) = \sqrt{\left(\sum_{i=1}^{n} (X_i - Y_i)^2\right)}, \text{ where } i = 1n$	(1)
2.	Squared Euclidean Distance	$D_{Ed}(X,Y) = \sum_{i=1}^{n} X_i - Y_i ^2$ where $i = 1 n$,	(2)
3.	City Block Distance	$D_{CBd}(X,Y) = \sum_{i=1}^{n} X_i - Y_i $, where $i = 1n$	(3)
4.	Minkowski Distance,	$D_{Mkd}(X,Y) = \left(\sum_{i=1}^{n} X_i - Y_i ^p\right)^{1/p}, \text{ where } i = 1n$	(4)
5.	Chebyshev Distance	$D_{Chebd}(X,Y) = \max_{i} X_i - Y_i $, where $i = 1n$	(5)
6.	Exponential Similarity Measure	$D_{ESM}(X_i, Y_i) = \sum_{i=1}^{n} \frac{ X_i - Y_i }{1 + e^{- X_i - Y_i }}, \text{ where } i = 1 \dots n$	(6)

7. P-Inverse Similarity
$$D_{Mkd}(X,Y) = \left(\sum_{i=1}^{n} |X_{i} - Y_{i}|^{2}\right)^{\frac{1}{4}}, \text{ where } i = 1 \dots n$$
8. Camberra Similarity
$$C(x,y) = \sum_{i=1}^{n} \frac{|X_{i} - Y_{i}|}{|x_{i} + y_{i}|}, \text{ where } i = 1 \dots n$$
9. Max-Min Similarity Measure
$$D_{MMM}(X,Y) = \sum_{i=1}^{n} \frac{\min(X_{i},Y_{i})}{|x_{i} + y_{i}|}, \text{ where } i = 1 \dots n$$
10. Geometric Average Minimum Similarity
$$GA_{Min}(X,Y) = \sum_{i=1}^{n} \frac{\min(X_{i},Y_{i})}{|x_{i} + y_{i}|}, \text{ where } i = 1 \dots n$$
11. Geometric Average Maximum Similarity
$$GA_{Max}(X,Y) = \sum_{i=1}^{n} \frac{Max}{|x_{i} + y_{i}|^{\frac{n}{2}}}, \text{ where } i = 1 \dots n$$
12. Cosine Amplitude Similarity
$$F_{i,j} = \frac{\left|\sum_{i=1}^{n} Max(X_{i},Y_{i})\right|}{\sqrt{\left(\sum_{i=1}^{n} x_{i}^{2} + \sum_{i=1}^{n} \left|\sum_{i=1}^{n} \left|x_{i}^{2} - \sum_{i=1}^{n} \left|$$

3. Engineering Materials Database(EMD)

It is a group of related records of engineering materials data set. Each record or an object is a group of related attributes of materials. The attributes of materials are the characteristics or behaviour of synthesized materials and these are measured by design engineer and manufacturing industries following the industrial standards. Data related to engineering materials are gathered from different information sources that include materials handbook [18] scientific literature[19] and Internet WebPages www.matweb.com. Information structure for organizing these gathered data are organized with scheme of Object Oriented Data Model .

4. PERFORMANCE INDEX MEASURE(PIM) FOR MATERIAL SELECTION

Performance index measure is proposed for the selection of the best among the similar materials. Performance Index Measure is the logical difference between the absolute aggregated values of attribute/characteristics of target material and its matching material. The best material is the one whose performance index measure value is the minimum among the most similar materials. Let $X_i = \{x_{i,1}, x_{i,2}, x_{i,3}, x_{i,4}, x_{i,5}, \dots, x_{i,n}\}$ and $Y_i = \{y_{i,1}, y_{i,2}, y_{i,3}, y_{i,4}, y_{i,5}, \dots, y_{i,n}\}$ be a target material and matching material respectively. PIM is mathematically expressed as

$$PIM(X,Y) = \sum_{i=1}^{n} |x_i| - \sum_{i=1}^{n} |y_i|$$
(14)

The best materials, whose Minimum Performance Index Measure(MPIM) value matches the target materials is defined by

$$MPIM(X,Y) = \min_{j=1}^{m} \left(\sum_{i=1}^{n} |x_i| - \sum_{i=1}^{n} |y_i| \right)$$
 (15)

4.1 Normalized Measures

Normalization is the mechanism for transforming measure values to another range normally -1 to +1. Normalization of PIM and SM values of similar materials are required to make relative comparison in decision making on material selection. Normalized Performance Index Measure is defined to transform PIM values to unique range.

$$NPIM = 1 - \frac{PIMXY_j}{Max(PIMXY)}$$
 (16)

where, PIMXY is the performance index value of X and Y. and Max(PIMXY) is the maximum Performance Index value among the similar materials.

$$NSM = 1 - \frac{Y_j}{Max(Y)} \tag{17}$$

where Yj is the distance/similarity measure values, Max(Y) is the maximum similarity value among the materials similarity measure values.

4.2 Algorithm For Similar Material Selection

Input: Target Material (TM): $X_i = \{x_{i,1}, x_{i,2}, x_{i,4}, x_{i,5}, \dots, x_{i,n}\}$, Materials Database(MD) Output: A List of materials Material matches the target materials

Method:

X, Y

```
1.
   Start
        PMX = Call \ PERFORMANCE\_MEASURE\_FUNCTION(X) //Calculates \sum_{i=1}^{n} |x_i|
2.
        Y [] = Call SIMILARITY-FUNCTION(SM[],TM, MD) // Function gives top ten similarity
3.
    materials
4.
5.
           for j=1 to m do
6.
                PMY[j] = Call PERFORMANCE_MEASURE_FUNCTION (Y[j]) // Calculates
7.
8.
                                                                 // PMY Performance Measure of Y
                                                         // PIM = Performance Index Measure
9.
                PIMX Y[j]) = PMX - PMY[j]
10.
11.
12.
          For j=1 to m do // Normalization of Measured Values
13.
14.
          Begin
               NPIMXY[j] = 1 - \frac{PIMXY_j}{Max(PIMXY)} // NPIMXY = Normalized Performance Index of
15.
```

```
NY[j] = 1 - \frac{Y_j}{Max(Y)}
                                                  // NY = Normalized Measured Value
16.
17.
          End
18.
19.
           //Selection of a Material
20.
21.
            MNPIMXY = 0
22.
               for j=1 to m do
23.
                 if (NPIMXY[j] > MNPIMXY) then
                                                      // MNPIMXY = Max of Normalized Performance
   Index
                                 MNPIMXY = PIMXY[j]
24.
25.
    Stop
```

5. EXPERIMENTAL RESULTS

In this experiment, Materials Database(MD) consisting of 5670 data sets of metal, ceramic and polymer type is considered for the selection of materials that very similar to target material features set, say X. A target material has several attributes that include maximum of 25 various kinds of properties as shown in table 2.

Table 2. Target Material Properties with values

TS	YS	MP	CS	IS	HRDS	TM	CS	MUT	DNSTY	ELGN	MACHN	CE
122	230	921	80	5	765	100	3	52	0.90	81	3	5
TCE	FS	WA	EI	CR	CORR	SM	СН	EXTRN	MOLD	CAST	MANFT	
3	3	1	1	2	2	5	4	5	3	5	2	

Each similarity function is applied for measuring the logical separation between the target and a material data set in the database. Top ten materials that are very closer to the target materials are considered and the relative Performance Index Measure(PIM) with all the materials data set is computed for material selection. A material whose behaviour similarity is closure to the behaviour of the target material is considered as the selected material.

The procedure is experimented with each similarity/distance function listed in the table 1. Experimental results corresponding to each function are depicted in figure from 1 to 13. In each graphical representation, similar group of materials are plotted along the X-axis and the normalized similarity measure values and the normalized performance index measure values are plotted along the Y-axis. The least normalized logical distance(The highest similarity) and the highest normalized performance index measure are considered as materials selection measures. Several similarity measure functions are deployed for material selection. Materials selected by different methods, their normalized similarity measure values and normalized performance index measure are tabulated in the table 3. Graphical representation of mined data are depicted in the figure 14. From the figure14, it is depicted that material M-7 is the ideal material for the target material since this has been commonly selected by six distance/similarity functions.

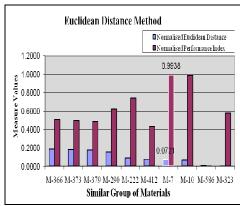


Figure 1. Performance measures of Similar Group of materials retrieved throug Euclidian distance function

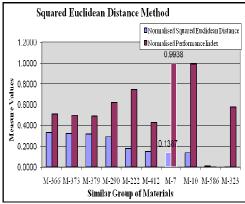


Figure 2. Performance measures of Similar Group of materials retrieved throug Sqauired Eucledian distance function

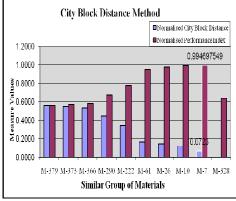


Figure 3 .Performance measures of Similar Group of materials retrieved throug City Block Ditance function

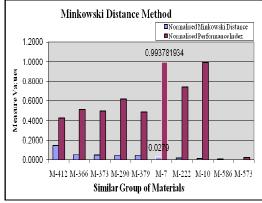


Figure 4 .Performance measures of Similar Group of materials retrieved throug Mickowski Distance Function

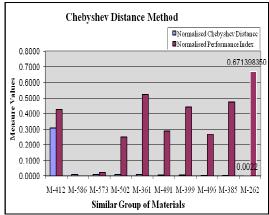


Figure 5 .Performance measures of Similar Group of materials retrieved throug Chebyshev Distance function

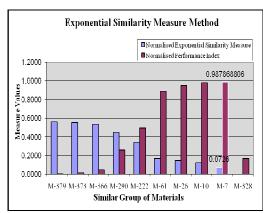


Figure 6 .Performance measures of Similar Group of materials retrieved through exponetial similarity Measure function

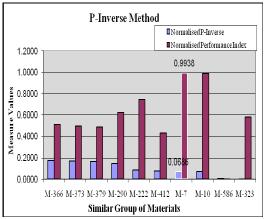


Figure 7 .Performance measures of Similar Group of materials retrieved throug Mickowski Distance Function.

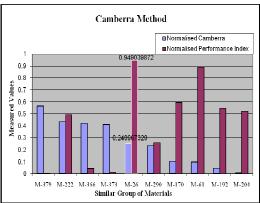


Figure 8. Performance measures of Similar Group of materials retrieved throug camberrral Function.

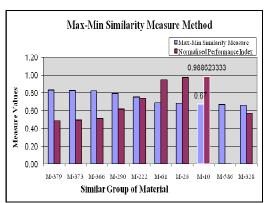


Figure 9.Performance measures of Similar Group of materials retrieved through Max-Min Similarity Function.

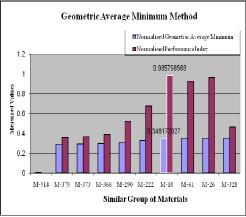


Figure 10 . Performance measures of Similar Group of materials retrieved through Geometric Average Minimum Function.

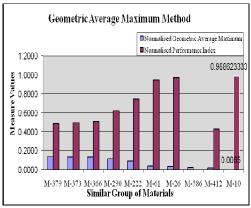


Figure 11. Performance measures of Similar Group of materials retrieved through Geometric Average Maximum Function.

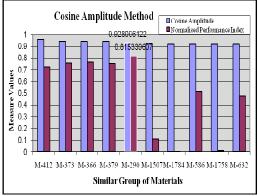


Figure 12 . Performance measures of Similar Group of materials retrieved through Cosine Appritute Function.

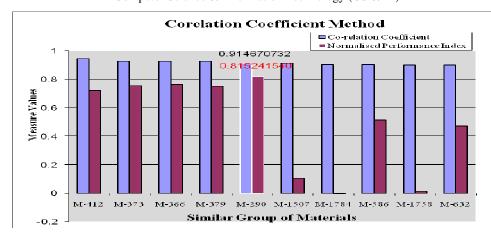


Figure 13 . Performance measures of Similar Group of materials retrieved through Correlation Coeefficent Method

 $\begin{tabular}{ll} Table 3. Material selection through similarity measure functions and on normalized Performance \\ Index Measure \\ \end{tabular}$

Methods	Similarity Measures	Selected Material	Normalized Measured Values	Normalized Performance Index
1	Euclidean Distance	M-7	0.072133127	0.993781934
2	Squared Euclidean Distance	M-7	0.138720149	0.993781934
3	City Block Distance	M-7	0.072336620	0.994697549
4	Minkowski Distance,	M-7	0.02788523	0.993781934
5	Chebyshev Distance	M-262	0.00221239	0.67139835
6	Exponential Similarity Measure	M-7	0.072559289	0.987868806
7	P-Inverse Similarity	M-7	0.068632226	0.993781934
8	Camberra Similarity	M-26	0.24896733	0.949039872
9	Max-Min Similarity Measure	M-10	0.67304755	0.988623333
10	Geometric Average Minimum Similarity	M-10	0.346172027	0.985798568
11	Geometric Average Maximum Similarity	M-10	0.006477780	0.988623333
12	Cosine Amplitude Similarity	M-290	0.92800612	0.815339607
13	Correlation Coefficient Similarity	M-290	0.91467073	0.81524154

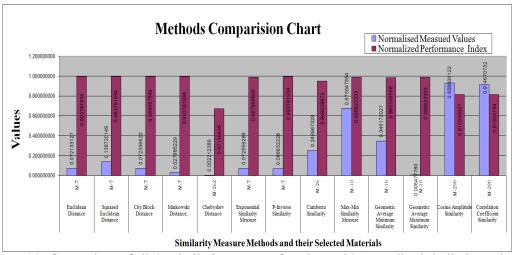


Figure 14. Comparison of all the similarity measure functions with normalized similarity and Performance Index Measure(PIM) values

6. CONCLUSION AND FUTURE SCOPE

In this paper similarity measures functionalities are used to select a required material, Before applying the similarity measure functions the dataset is properly classified into metals, polymers and ceramics using some techniques of classifications in data mining. Hence proposed a model for retrieving selective information from the vast amount of data using similarity measure functions. Systematic study of various similarity measure functions on engineering materials database is done. The material which gives a high performance index value and less distance between selected and target material is determined as an ideal material. The proposed approach is suitable for the selection of engineering materials that suit for the required materials design requirement specifications. Thus can overcome the haphazardly selecting the materials in materials design and manufacturing industries.

Further it proposed to find a model which would be the exact ideal distance or similarity function for the selection of materials that suit for complex applications in real empirical world. and also the computational complexity such as time complexity and space complexity can be examined for the model.

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