

THE JÖRESKOG TECHNIQUE APPLIED FOR MATERIALS DESIGN

Constantin TÂRCOLEA, Adrian PARIS

Abstract: *In the design process the choice of materials for a new product is made from a very large spectrum. In practice the rigorous methods of materials' classification are made according to their attributes. Based on the principal component analysis, the observable variables are related only to a few artificial factors. The retained variance of the original cloud of different materials is maximal by this new representation. The Jöreskog' technique is used for the dimensional reduction in a bivariate subspace for a family of materials.*

Key words: *principal component analysis, materials selection, artificial factors, design of experiments.*

1. INTRODUCTION

“The goal of design is create products that perform their function effectively, safely, at acceptable cost” (Ashby, 1999) [1].

The choice of a material for a product is not based on all the attributes, is based on a combination of properties. In this paper it is presented a method of reduction of attributes to a combination of a few artificial factors.

The selection of the materials group is based on the following premises:

- the taking into consideration of an ever larger spectrum of materials, otherwise expressed, defining as complete as possible the selection range;
- the division of materials in "equivalence classes" otherwise expressed as the classification of materials thus obtaining a significant reduction of the selection space, the initial chaotically multitude is reduced to smaller number of classes, the number of each class having common properties, processes accompanied or not by the elimination or some materials taken into consideration;
- the establishing of the same simple and efficient methods of selection, with the possibility of implementing on a computer.

A possibility of getting down the properties range is the taking into consideration of the correlation between the properties, studying thus only a few independent properties to the possible extent.

The introduction of the up-to-date calculation enables the data stocking concerning the properties, from the standard version, under the normal temperature and the time $t = 0$, up to more complete versions, taking into account their variability as against the temperature, time, etc. [3].

An inventory of materials is necessary to be made in parallel, considering even the technological versions of the materials obtained for example by settling (dying, galvanizing, diffusion, plating, etc.).

The classification of materials is often empirically made, for example in six groups [2, 3] metallic materials, polymers, elastomers, glasses, ceramics and compound materials. Another variant [3] uses as criterion

the cristallinity of materials (crystalline or non-crystalline and compound) each class being grouped in underclasses as per the structure type, way of obtaining etc. This classification can be developed in underclasses of common materials (cast irons, steels, aluminum alloys, etc.) and is extended to the types from each of the underclasses [4].

From all those herein above, its results the need of substantiating of some rigorous analytical methods of materials' classification according to their properties.

2. DISPLAYING MATERIAL PROPERTIES

The properties of engineering materials have a characteristic span of values. The span can be large: many properties have values which range over five or more decades. Upon Ashby one way of displaying this is as a bar-chart like that of Fig. 1 for thermal conductivity [1]. Each bar represents a single material.

The length of the bar shows the range of conductivity exhibited by that material in its various forms.

The materials are segregated by class. Each class shows a characteristic range: metals have high conductivities; polymers have low; ceramics have a wide range, from low to high.

Much more information is displayed by an alternative way of plotting properties, illustrated in the schematic of Fig. 2 [1].

Here, one property (the Young's modulus, E , in this case) is plotted against another (the density, ρ) on logarithmic scales.

The range of the axes is chosen to include all materials, from the lightest, flimsiest foams to the stiffest, heaviest metals. It is then found that data for a given class of materials (polymers for example) cluster together on the chart; the *sub-range* associated with one material class is, in all cases, much smaller than the full range of that property.

Data for one class can be enclosed in a property envelope, as the figure shows. The envelope encloses all members of the class.

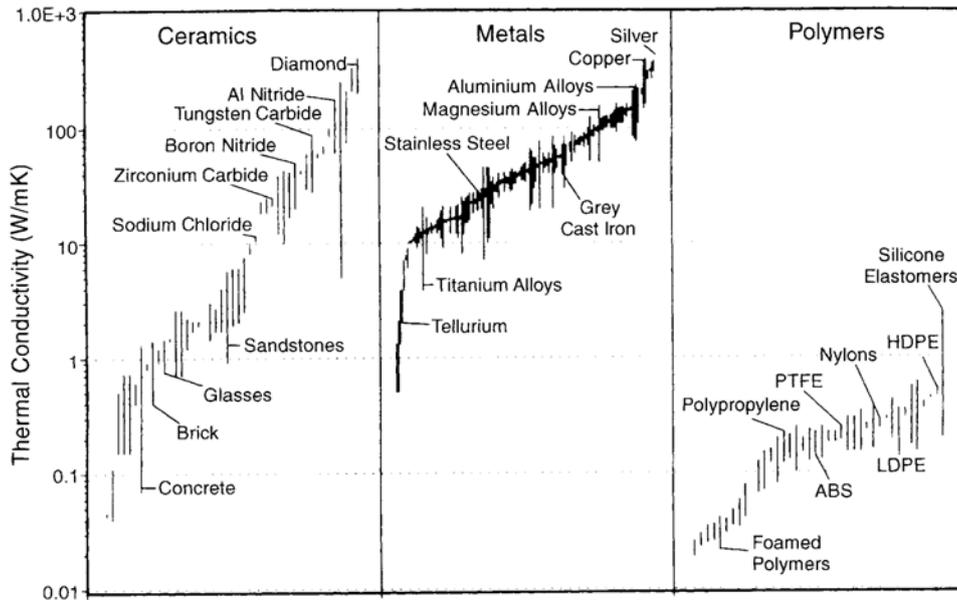


Fig. 1. Bar-chart display of materials properties.

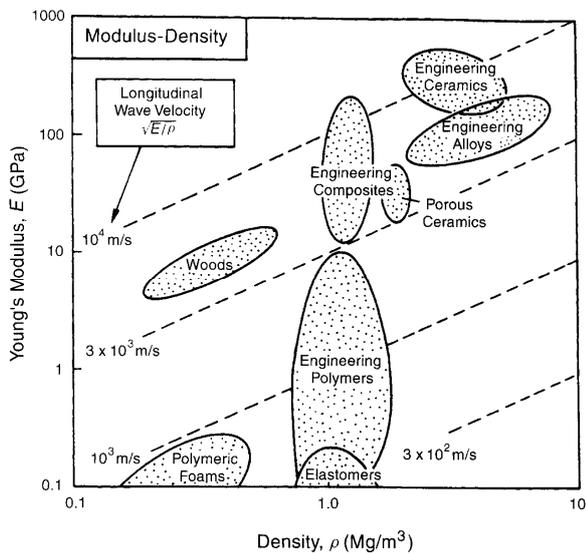


Fig. 2. Bidimensional plotting of materials properties.

3. AN APPLICATION OF PCA BASED ON JÖRESKOG METHOD

Principal component analysis (PCA) is a standard technique to reduce multivariate data sets to lower dimensions [5].

The number of observable attributes gives the dimension of the initial vector space of the objects. The PCA model represents the objects in view in a strictly subspace [6].

Instead of reale attributes the PCA proposes new factors, but artificial ones, so that the subspace yields the minimum deformation of the original cloud. In the present paper the dimensional reduction for a family of materials uses the Jöreskog' method [7, 8].

Let us consider X as a 6x9 dimensional matrix, attributes/materials constructed for the first six attributes from Table 1 [9].

The standardized matrix associated with X is matrix Z.

Table 1

Properties and materials for sliding bearing [9]

Materials	Alloys on the basis of		Bronze on the basis of		Aluminum Alloys			Porous sintered bearings		Plastics	Artificial carbon
	Lead	Tin	Lead	Tin	Al						
Sliding properties	1	2	3	3	3	2.5	3.5	4	4		
Embeddability	1	2	3	3	3	2.5	3	4	5		
Emergency running (antifrictionnal) properties	1	2	2	3	2	2	1	1	1		
Loadability	4	3	2	2	2	2	3	4	5		
Heat conduction /thermal expansion	4	4	3	3	3	2	4	5	5		
Corrosion resistance	5	3	4	3	2	2	3.5	3	2		
Minimal or dry lubrication	2	3	4	5	4	3	1	1	1		

$$X = \begin{pmatrix} 1 & 2 & 3 & 3 & 3 & 2.5 & 3.5 & 4 & 4 \\ 1 & 2 & 3 & 3 & 3 & 2.5 & 3 & 4 & 5 \\ 1 & 2 & 2 & 3 & 2 & 2 & 1 & 1 & 1 \\ 4 & 3 & 2 & 2 & 2 & 2 & 3 & 4 & 5 \\ 4 & 4 & 3 & 3 & 3 & 2 & 4 & 5 & 5 \\ 5 & 3 & 4 & 3 & 2 & 2 & 3.5 & 3 & 2 \end{pmatrix},$$

$$Z = \begin{pmatrix} -1.96 & -0.92 & 0.11 & 0.11 & 0.11 & -0.40 & 0.63 & 1.15 & 1.15 \\ -1.72 & -0.83 & 0.05 & 0.05 & 0.05 & -0.39 & 0.05 & 0.93 & 1.82 \\ -0.94 & 0.47 & 0.47 & 1.88 & 0.47 & 0.47 & -0.94 & -0.94 & -0.94 \\ 0.89 & 0 & -0.89 & -0.89 & -0.89 & -0.89 & 0 & 0.89 & 1.79 \\ 0.33 & 0.33 & -0.66 & -0.66 & -1.66 & 0.33 & 1.33 & 1.33 & 1.33 \\ 1.92 & -0.05 & 0.93 & -0.05 & -1.04 & -1.04 & 0.44 & -0.05 & -1.04 \end{pmatrix}.$$

Using the matrix equation:

$$R = \frac{1}{8} Z * Z_{rr}, \tag{1}$$

it results that:

$$R = \begin{pmatrix} 1 & 0.94 & -0.15 & 0.17 & 0.34 & -0.54 \\ 0.94 & 1 & -0.18 & 0.34 & 0.42 & -0.59 \\ -0.15 & -0.18 & 1 & -0.79 & 0.71 & -0.23 \\ 0.17 & 0.34 & -0.79 & 1 & 0.89 & 0.11 \\ 0.34 & 0.42 & 0.71 & 0.89 & 1 & 0.14 \\ -0.54 & -0.59 & -0.23 & 0.11 & 0.14 & 1 \end{pmatrix},$$

which is the correlation matrix. The proximity between attributes is expressed in terms of correlations.

The inverse matrix of R is:

$$R^{-1} = \begin{pmatrix} 403 & -4002 & 1113 & 2949 & -1542 & -0.65 \\ -4002 & 4247 & -11 & -2863 & 13.35 & 2.49 \\ 1113 & -11 & 5.91 & 10.43 & -4.39 & 0.28 \\ 2949 & -2863 & 10.43 & 2858 & -16.33 & 0.4 \\ -1542 & 13.35 & -4.39 & -16.33 & 12.39 & -1.33 \\ -0.65 & 2.49 & 0.28 & 0.4 & -1.33 & 2.35 \end{pmatrix},$$

it obtains:

$$\text{diag}(R^{-1}) = \text{diag}(40.3; 42.47; 5.81; 28.58; 12.39; 2.35),$$

$$(\text{diag}(R^{-1}))^{\frac{1}{2}} = \text{diag}(6.35; 6.52; 2.43; 5.35; 3.52; 1.53),$$

$$(\text{diag}(R^{-1}))^{-1} = \text{diag}(0.025; 0.024; 0.17; 0.035; 0.08; 0.43).$$

Jöreskog's method considers that theoretical covariance matrix of the standardized attributes, V, is factorized as:

$$V = L_r * L + \text{diag}(s_1^2, \dots, s_6^2). \tag{2}$$

For the uniqueness of the estimators of the matrices from the decomposition of V it is supposed that the

variances are direct proportional with the inverse values of the diagonal elements of the matrix V⁻¹; that is:

$$\text{diag}(s_1^2, \dots, s_6^2) = m(\text{diag}(V^{-1}))^{-1}, \tag{3}$$

where m is the proportional parameter.

Further on, it is denoted by R* the following matrix:

$$R^* = \text{diag}(R^{-1})^{\frac{1}{2}} * R * \text{diag}(R^{-1})^{\frac{1}{2}}. \tag{4}$$

It obtains:

$$R^* = \begin{pmatrix} 4029 & 39 & -2.36 & 5.92 & 7.75 & -5.23 \\ 39 & 4247 & -2.89 & 1206 & 9.72 & -5.96 \\ -2.36 & -2.89 & 5.9 & -10.27 & -6.05 & -0.86 \\ 5.92 & 1206 & -10.27 & 2858 & 16.83 & 0.9 \\ 7.75 & 9.72 & -6.05 & 16.83 & 12.38 & 0.77 \\ -5.23 & -5.96 & -0.86 & 0.9 & 0.77 & 2.35 \end{pmatrix}.$$

The eigenvalues [10] of this matrix are given in the Table 2 and the first two eigenvectors in the Table 3.

Because:

$$\frac{\lambda_1 + \lambda_2}{\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 + \lambda_6} = 0.954 > 0.95,$$

it can be considered only the 2-dimensional subspace.

An estimator for the parameter m is the average of the remained eigenvalues:

$$\hat{m} = \frac{1}{4}(\lambda_3 + \lambda_4 + \lambda_5 + \lambda_6) = 1.5071.$$

The parameters of interest are the variances, given by:

$$s_i^2 = \frac{\hat{m}}{r_{ii}}, \quad i \in \overline{1,6}, \tag{5}$$

where r_{ii} is the element ii of the matrix R⁻¹.

Table 2
Eigenvalues of the matrix R*

Eigenvalues
λ ₁ = 88.19
λ ₂ = 36.92
λ ₃ = 3.63
λ ₄ = 0.25
λ ₅ = 2.14
λ ₆ = 0.84

Table 3
The values of the first two eigenvectors of the matrix R*

v ₁	v ₂
-0.634262594	0.321658498
-0.676926524	0.175405541
0.091808859	0.298073488
-0.276539771	-0.76157364
-0.219542078	-0.428352389
0.079872452	-0.115934142

In our case it is obtained the values of s_i^2 , which are given in Table 4.

Further on, it should be calculate:

$$k_i^2 = 1 - s_i^2, i \in \overline{1,6}. \tag{6}$$

The results are given in the Table 5.

The two eigenvectors, denoted as T, U , associated with the first two chosen eigenvalues are determined so that:

$$\|T\|^2 = \lambda_1 - \hat{m}, \|U\|^2 = \lambda_2 - \hat{m}. \tag{7}$$

The matrix of these eigenvectors is matrix A :

$$A = \begin{pmatrix} -5.91 & 1.91 \\ -6.3 & 1.04 \\ 0.85 & 1.77 \\ -2.57 & -4.53 \\ -2.04 & -2.55 \\ 0.74 & -0.69 \end{pmatrix}.$$

In the next step it is obtained the loading matrix:

$$L = (\text{diag}(R^{-1}))^{\frac{1}{2}} \times A, \tag{8}$$

$$L = \begin{pmatrix} -0.93 & 1.91 \\ -0.97 & 0.16 \\ 0.35 & 0.73 \\ -0.48 & -0.85 \\ -2.04 & -2.55 \\ 0.74 & -0.69 \end{pmatrix}.$$

It results:

$$k_i^2 \cong l_{i1}^2 + l_{i2}^2, \text{ for } i \in \overline{1,6}, \tag{9}$$

which confirm the correctness of the model.

Table 4

Values of s_i^2
0.037401
0.035487
0.255196
0.052734
0.121682
0.641638

Table 5

Values of k_i^2
0.962599
0.964513
0.744804
0.947266
0.878318
0.358362

Now should be calculated the correlations between every eigenvector and the original attributes respectively. The results can show a strong positive/negative correlation between the first/second eigenvector, and same initial properties.

4. CONCLUSIONS

The first part of the paper presents a few general considerations concerning the methods of materials selection in design process. Further on the Ashby' idea to visualize the materials properties as bidimensional charts is developed for a wider range of properties.

A possibility to reduce the number of attributes of materials in the design is the PCA model, based on Jöreskog' method.

In the present research it is used a bivariate artificial subspace for the considerate range of materials. The real attributes of each object can be expressed with a good precision as function of artificial axes.

The application of this model will simplifies the materials design and there are many other possible extensions in the design process. Further more, a mixture between Jöreskog' method and materials design principles is useful through future developments.

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Authors:

PhD Math., Constantin Târcolea, Professor, University "Politehnica" of Bucharest, Department of Mathematics, E-mail:constantin_tarcolea@yahoo.com
 Eng. Adrian Paris, Lecturer, University "Politehnica" of Bucharest, Materials Tehnology and Welding Department, E-mail: adrianparis@amza.camis.pub.ro