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# A TECHNIQUE FOR QUANTITATIVE DESCRIPTION OF PARTICLE'S SPATIAL STRUCTURE IN A DEFINED FEATURE SPACE

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## ABSTRACT

A particle systematic section features supply a basis for description of particle's spatial structure in a defined feature space. A similarity of the particle sections in the space can then be evaluated by using a minimum spanning tree algorithm. A partition of the spanning tree provides a systematic technique for the quantitative description of particles.

Key words: image analysis, order, minimum spanning tree, particle spatial structure, partition, systematic sections.

## INTRODUCTION

Analysis of spatial organization of particles allows us to explain their physical properties in a more precise way. At the present time, however, it seems impossible to make it without previous selection of features describing particle morphological structure. Systematic sections provide a basis for analysis of particle's spatial structure in a defined feature space. In this paper, we show a relation to a method of image analysis based on a distance function in a defined space of particle features. The value of the distance function corresponds to a measure of similarity between particle sections in the space, and can be applied for quantitative studies of the structural changes of particles. In particular, the presented technique allows us to take a decision on a random or non-random character of particle's spatial organization.

## ASSUMPTIONS AND NOTATION

Let us assume that a particle is represented by a stack of its n systematic sections. Two particle sections $U_i$ and $U_j$ are called the sections at the same particle level if $j = n-i+1$ . Furthermore, let level $(U_i)$ denote the particle level corresponding with the section $U_i$. Thus,

$$\text{level}(U_i) = \begin{cases} i & \text{for } i=1, \ldots, r \\ n-i+1 & \text{for } i=r+1, \ldots, n \end{cases} \tag{1}$$

where $r=n/2$ if $n$ is even, and $r=(n+1)/2$ if $n$ is odd. Each $U_i$ section is described by $p$ features (e.g. geometric properties), and is represented by the vector

$$U_i=(x_{i1}, \ldots, x_{ik}, \ldots, x_{ip}), \tag{2}$$

where $x_{ik}$ denotes the value of the kth feature of section $U_i$.

The distance function is a measure of similarity of particle sections in the space. Then, let us assume, that any two particle sections $U_i$ and $U_j$ can be called similar patterns in the defined feature space if and only if the distance $d_{ij}$ between them will be less than a treshold distance $t$. The problem is to map the particle sections with respect to the plane of "symmetry" by means of their similarity in the defined feature space. Then, we need to take into account a similarity between the sections $U_i$ and $U_{n-i+1}$ in the space. If these sections are not similar, then they should not be mapped into themself with respect to the plane of "symmetry" intersecting a central region of the particle in the cutting direction. Therefore, we should consider a similarity of sections at the same particle level in the defined feature space under an assumed criterion. To this end, we align a sequence of all systematic sections of the particle under the rule of the nearest distance.

BASIC TOOLS

Let us study a particle's spatial structure in a defined feature space by using minimum spanning tree. A distance matrix $D=(d_{ij})$ (of order $n \times n$) represents a complete weighted graph $G=(U, E)$. The set $U$ of particle sections represents the set of the graph vertices, whereas the set $E$ is the set of graph edges. The value of the distance between sections $U_i$ and $U_j$ is a weight of the edge $e_i=(U_i, U_j)$. Further, we need to find a spanning subgraph of graph $G$, in which the total weight of edges is minimal. Minimum spanning tree $MST=(U, F)$ satisfies such property ($F \subset E$). Then, MST represents a form of ordering of particle sections. We want to study, whether the sections at the same or the neighbouring particle level show most similar features in the defined space. Then, we need to consider, whether all MST edges $e_i=(U_i, U_j)$ satisfy the following requirement:

$$j=i+1 \quad \text{or} \quad j=n-i \quad \text{or} \quad j=n-i+1 \tag{3}$$

In order to find MST edges satisfying the requirement (3) we can apply an algorithm of tree partition (Kaczmarek, 1989). The result of this algorithm is a partition of the n-element set

$U=(U_1, \dots, U_n)$. This partition is a collection of subsets $S_i$ of the set U such that $S_i \cap S_j = \emptyset$ and $\bigcup_{i=1}^{q} S_i = U$. Then, we partition $n=\sum_{i=1}^{q} n_i$ vertices into q classes, the ith class contains $n_i$ vertices. Every one subset $S_i$ in the partition U represents the MST vertices connected by edges satisfying the requirement (3). In addition, the edge weights in the subtrees of MST are less than a treshold value $t$. However, we need to find the number of ways of vertex set partition into q subsets. Let P={ partition of n into q parts }. The question arises of the number P(q, n) of unordered ways of writing the number n as the sum of exactly q positive integers, i.e.

$$P(n, q)=\left|\{(n_1, n_2, \dots, n_q): \text{each } n_i \text{ is a positive integer}, \sum_{i=1}^{q} n_i=n, \text{ and } n_1 \geq n_2 \geq \dots \geq n_q \geq 1\}\right| . \tag{4}$$

Given a partition $n=(n_1, n_2, \dots, n_q)$ we can represent each part by the appropriate number of points in q rows ($n_i$ points in ith row). This form of partition presentation is called Ferrer diagram, and can be used to prove a simple recurrence formula for P(q, n) (see Constantine , 1987):

$$P(n, q)= \sum_{i=1} P(n-q, i) \quad \text{for} \quad n \geq q \geq 0 . \tag{5}$$

We assume that P(0, 0)=0, P(n, 0)=0 for n>0, and P(n, k)=0 for n<k. The number of ways of presenting n as the sum of 1 integers, or as the sum of n integers is unique, i.e. P(n, 1)=P(n, n-1)=P(n, n)=1. Of course, the number of partitions of n as the sum of an arbitrary number of parts is equal to:

$$P(n)= \sum_{q=0}^{n} P(n, q). \tag{6}$$

## OUTLINE OF THE TECHNIQUE FOR QUANTITATIVE ANALYSIS OF PARTICLE'S SPATIAL STRUCTURE IN A DEFINED FEATURE SPACE.

The technique presented in this paper is based mainly on three algorithms. At the first stage a similarity of particle section is analyzed by using a minimum spanninig tree algorithm (Bentley and Ottmann, 1981). Further, we shall partition MST. A tree partition algorithm (Kaczmarek, 1989) can be condensed as follows:

*step 1.* Assign the label 0 to the vertex $U_2$.

*step 2.* Find any unlabelled vertex $U_i$ which is connected with the labelled vertex of MST. Assign the label to the vertex $U_i$

if and only if the edge $e_i=(U_i, U_j)$ satisfies the requirement (3), and $d_{ij}<t$.

Repeat *step 2* until all MST vertices are labelled. Then, clusters of all vertices having the same labels are subtrees of the MST. This yields our required partition.

Subsequently, we need to enumerate a number of partitions of an integer P(n, q). To this end we can use the Hindenburg algorithm (Andrews, 1976) which can be summarized as follows:

*step 1.* At the beginning of the algorithm fix:

$$P(n, q)=(1, 1, \ldots, 1, n-q+1). \quad (7)$$

*step 2.* Find a greatest value j such that

$$n_q-n_j\geq 2 . \quad (8)$$

Given a partition $(n_1, n_2, \ldots, n_q)$ we define a new partition

$$(n_1', \ldots, n_q')=(n_1,\ldots, n_{j-1}, n_j+1, n_j+1,\ldots, n_j+1, n_q'), \quad (9)$$

where $$n_q'=n-\sum_{i=1}^{q-1} n_i'. \quad (10)$$

Repeat *step 2* until the requirement (8) is satisfied.

EXAMPLES

Two particles observed in systematic sections will be presented to illustrate the technique. The following features have been measured on particle sections: area and perimeter of the particle , area and perimeter of a selected particle subunit (Table 1). The matrix of normalized Euclidean distances has been formed on the basis of measurements on each particle. Thus, a similarity of particle sections can be considered by using a tree partition algorithm (Figure 1). The treshold value of the distance has been calculated by using the following formula:

$$t = \frac{1}{n}\sum_{j=1}^{n} \min_i d_{ij}.$$

In our case, sections $U_i$ and $U_j$ can be treated as similar if $d_{ij}<t$ ($t$=0.25 for particles A and B). Subsequently, using the tree partition algorithm, the following subsets of sections have been determined for:

particle A

$S_1=\{U_1, U_2, U_8, U_9\}$, $S_2=\{U_3, U_6, U_7\}$, $S_3=\{U_4\}$, $S_4=\{U_5\}$,

and particle B

$S_1=\{U_1, U_9\}$, $S_2=\{U_2, U_8\}$, $S_3=\{U_3, U_4, U_6, U_7\}$, $S_4=\{U_5\}$.

Thus, both particles have been partitioned into 4 parts.

Table 1. Features of systematic sections of particles A and B. (at a magnification of 7000x)

| $U_i$ | Area of particle section ($mm^2$) | Perimeter of particle (mm) | Area of particle subunit ($mm^2$) | Perimeter of particle subunit (mm) |
|---|---|---|---|---|
| Particle A | | | | |
| $U_1$ | 234 | 67 | 70 | 57 |
| $U_2$ | 346 | 87 | 82 | 87 |
| $U_3$ | 544 | 115 | 187 | 116 |
| $U_4$ | 665 | 98 | 302 | 141 |
| $U_5$ | 811 | 110 | 485 | 208 |
| $U_6$ | 638 | 99 | 171 | 71 |
| $U_7$ | 476 | 90 | 130 | 64 |
| $U_8$ | 312 | 90 | 56 | 50 |
| $U_9$ | 218 | 65 | 26 | 21 |
| Particle B | | | | |
| $U_1$ | 296 | 92 | 92 | 97 |
| $U_2$ | 526 | 107 | 276 | 116 |
| $U_3$ | 806 | 133 | 318 | 160 |
| $U_4$ | 640 | 124 | 314 | 184 |
| $U_5$ | 922 | 148 | 350 | 221 |
| $U_6$ | 756 | 146 | 314 | 216 |
| $U_7$ | 700 | 129 | 240 | 180 |
| $U_8$ | 480 | 115 | 270 | 151 |
| $U_9$ | 242 | 73 | 60 | 56 |

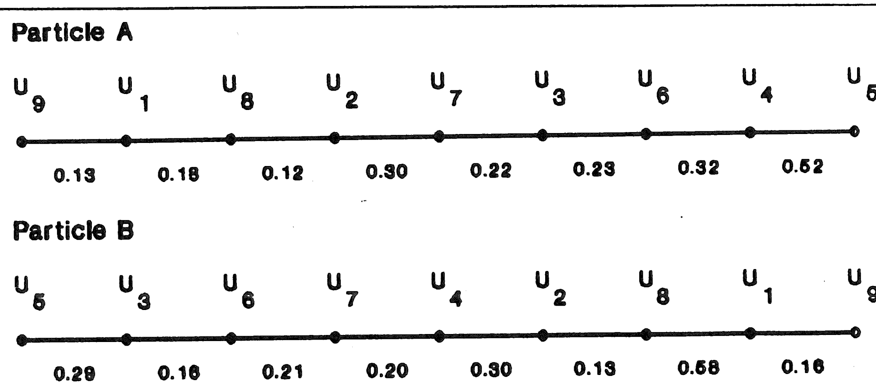


Figure 1. Minimum spanning trees formed for particles A and B. The $U_i$ indicate particle section, the figures between them denote the distances.

Furthermore, we enumerate the number of unordered ways of partition P(n, q) by using Hindenburg algorithm, P(9, 4)=6.

## APPLICATION

The method presented in this paper allows us to study a spatial structure of particles in a defined feature spaces. However, the results of the analysis depend mainly on selected features, definition of the distance function in the space, and the assumed criterion of similarity between particle sections. Therefore, it is worth to consider when a particle structure is of a random or non-random character in the defined space. The procedure of tree partition results in subsets of vertices representing similar particle patterns under a certain criterion. Then, upon morphological studies of particles, we can note whether the partition happens to have the specified number of subsets. Let a number of subsets in a partition of MST be a random variable. Then, it is interesting to determine the distribution of the random variable. A statistical analysis of the distribution allows us to take a decision, whether the particle structure is random in the defined feature space. Moreover, we may compare the distributions of the random variable in the different spaces of features. Thus, the obtained results can be used for the quantitative description of morphological structure of particle, and even for an elaboration of particle models. The question arises of an advantage of the studies by using MST partition. An approach is to consider particles from a morphological point of view in the space, to study order and disorder in particle structure, and to conclude a random character of certain forms of particle structures. These results can be very useful for further classification of an investigated material. By using methods of cluster or discriminant analysis on the basis of measurements of particle sections, we can choose significant features of particles. However, we loose information about the mutual relations of features in several particles. In particular, this information can be important for studies of biological structures. That is why, in this paper, the method of multidimensional analysis for a particle has been presented in order to use the obtained results for further statistical analysis or modelling.

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