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ON THE DETERMINATION OF THE SHAPE-TYPE OF PARTICLES

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ABSTRACT

Based on observations on similar-looking randomly deformed particles inference is made about the original common shape-type of these particles by means of statistical tests.

Keywords: cross-sectional breadth, model selection by tests, random deformation, shape-type of grains.

INTRODUCTION

Quite often the outcome of an experimental investigation presents itself in the form of a set of different, disjoint, but to a certain extent similar particles in an Euclidean space $\mathscr{R}^k$. The near similarity of the particles suggests then to assume that the particles have arisen by individual random deformation applied to the contours of bodies of a parametric class of forms, which represents the shape-type of the typical particle. When constructing a suitable stochastic model explaining the genesis of the experimental outcome, an important task consists in reconstructing the original form of the particles. In the following we treat problems where a choice has to be made between a simple prototype form on one hand and a more complex alternative shape. Based on a few easily to perform measurements the perferred shape-type has to be selected in a way that incorrect decisions for the alternative shape-type are seldom and that under this restriction the choice of the alternative shape-type is most often recommended when it is actually preferable. It will be shown that statistical tests are useful tools in this context.

PROBLEM DESCRIPTION BY A DEFORMATION MODEL

Since most applications concern sets in dimension 2 and 3, our considerations will be restricted to planar particles in $\mathscr{R}^2$ or spatial particles in $\mathscr{R}^3$.

Under the null-hypothesis H_0 we specify the planar prototype to be rectangular and the spatial prototype to be a circular cylinder; under this hypothesis the grains have thus roughly the form of sticks. We are here concerned with experimental set-ups where the original shape is completely specified by a symmetry axis and by the cross-sectional breadth measured at the points along this symmetry axis, a set-description model proposed in Stoyan and Stoyan (1992). Note that in this paper the prototype shape is described by the thickness of the body measured orthogonally to the symmetry axis and not by the radius vector function as in Streit (1997; 2000; 2003; 2005; 2006). It is supposed that the axis of symmetry is recognizable either by means of landmarks or by taking into account a geometrical property of the particles (for instance that the axis of symmetry is coinciding with the axis of the diameter, thus with the axis of the segment of maximal length realized within the body). The particle-types chosen under H_0 are particularly simply structered in view of the fact that the cross-sectional breadth does not change along this axis. Under H_1 we consider basic shape-types which allow changes in cross-sectional breadth, choosing in the two-dimensional version of the problem:

- a circle — in case A
- an ellipse — in case B
- an isosceles triangle — in case C
- a particle bounded by the hyperbola $(x^2/a_H^2) - y^2 - 1 = 0$ and the straight-lines $y = -1/2$ and $y = +1/2$ (expressed in planar Cartesian coordinates $(x,y)'$) — in case D.

In the three-dimensional set-up the corresponding rotation-symmetric bodies represent the shape-types under H_1, that is to say we work with the assumption that the basic form is:

- a ball — in case A
- a rotations-symmetric ellipsoid — in case B
- a straight circular cone — in case C

- a rotation-symmetric hyperboloid bounded by the surfaces $((x^2+y^2)/a_H^2)-z^2-1=0$ and the planes $z=-1/2$ and $z=+1/2$ (expressed in Cartesian coordinates $(x,y,z)'$ in $\mathscr{R}^3$) in case D.

In our stochastic models certain features like the position, the size or the orientation of the particles are supposed independent of the shape and need therefore not to be taken into consideration. Each of the observed particles may thus be first reoriented and standardized by putting its axis of symmetry in vertical position and by assigning the ordinate $y=-1/2$ to its lowest point and the ordinate $y=1/2$ to its top in the planar case and proceeding analogously with the assignment of the z-values in the spatial case (should this operation admit different realisations we shall choose the one which leads to the largest value of the test statistic to be calculated). This standardization is carried out by using a unit of length in all length measurements for the same particle adjusted to produce this situation. For a fixed integer $n \in 2,3,....$ orthogonally to this axis the cross-sectional breadth is measured at the ordinate levels $y=-(n-1)/(2n)$,$y=-(n-2)/(2n),\ldots,y=(n-2)/(2n)$,$y=(n-1)/(2n)$ in the planar case, with y replaced by z and taking the straight line orthogonal to the z - axis which yields the largest value in the spatial case. Note that any of these level straight lines cuts the boundary of the prototype shape only in two points symmetrically arranged around the symmetry axis. n represents somehow the degree of measuring-effort undertaken per individual particle. Let N be the number of observed particles and $\vec{Q}=(Q^{(l)}(i/(2n))[i=-(n-1),\ldots,n-1;l=1,\ldots,N])'$ the set of measurements to be taken, where $Q^{(l)}(i/(2n))$ designates the cross-sectional breadth (*i.e.*, maximal thickness) at level $y=i/(2n)$ or $z=i/(2n)$ of the $l$the particle, $q^{(l)}(i/(2n))$ its realized value and $'$ the transposition of a matrix. Since our data set consists simply of an ordered set of length measurements it is sufficient to explain the effect of random deformation only at the ordinate levels where such mesurements are taken. We shall here assume that random deformation of a particle is caused by an individual dilatation of the cross-sectional breadth of each particle at each level of the ordinate. Thus random deformation is described by the following relations between the random variables of the competing stochastic models valid under H_0 respectively under H_1:

$$H_0 : Q^{(l)}(i/(2n)) = Y^{(l)}(i/(2n)) \cdot a \quad [i=-(n-1),\ldots,(n-1);l=1,\ldots,N] ,$$

and

$$H_1 : Q^{(l)}(i/(2n)) = Y^{(l)}(i/(2n)) \cdot a \cdot b(i/(2n)) \quad [i=-(n-1),\ldots,(n-1);l=1,\ldots,N] ,$$

where a designates the breadth of the rectangle respectively the cross-sectional breadth of the circular cylinder and $a \cdot b(i/(2n))$ the cross-sectional breadth of the prototype shape at ordinate level $y=i/(2n)$ respectively $z=i/(2n)$ under H_1. For $l \in 1,\ldots,N$, $(Y^{(l)}(i/(2n))\,[i=-(n-1),\ldots,n-1])'$ are supposed to be independent random samples from an exponential distribution with parameter λ.

Fig. 1 illustrates how the experimental data are obtained in the planar case for a axialsymmetric figure. The symmetry axis is vertical, the top point has planar coordinates $(0,1/2)$, the middle point of the lowest segment has planar coordinates $(0,-1/2)$, n is 5 and we thus take 9 measurements in determening the lengths of the horizontal arrows at levels $-4/10,-3/10,\ldots,4/10$. The observed particles are usally not any more axial-symmetric due to random deformation, but the length measurements can still be performed at the prescribed levels and the values of $Q^{(l)}(i/2n)$ be obtained in this way.

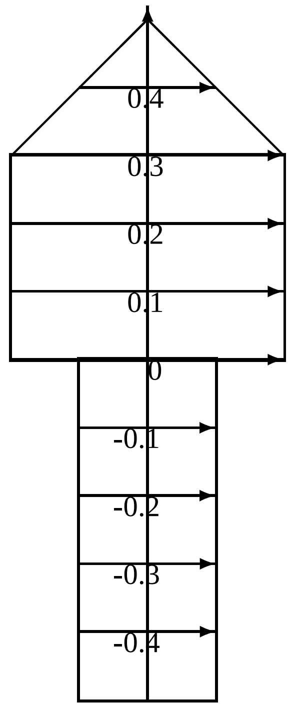

Fig. 1. *Measurements leading to the experimental data.*

Taking into account that the prototype shapes under H_0 and H_1 should give rise to the same observed particles, it is reasonable to ask that the following additional condition is fulfilled, whenever the family of shapes admitted under H_1 is indexed by at least two unrelated parameters specifying an individual figure within the shape-class:

The prototype shape under H_0 has in the planar case the same surface area as the prototype shape under H_1 and the prototype shape under H_0 has in the spatial case the same volume as the prototype shape under H_1.

Note that we are confronted here with a typical problem of stereology, since we would like to use one-dimensional measurements to find out the shape of a higher-dimensional set.

THE GENERAL DECISION RULE

We shall now apply standard test theory (Mukopadhyay, 2000) to determine the optimal (*i.e.*, most powerful) procedure, which allows us to decide if it is appropriate to adopt the shape of a stick (rectangular or cylindric) or whether in view of the measurements we should rather opt for the alternative shape-type admitted under H_1. In fact the measured lengths do not have the same chance to arise under the null hypothesis and under the alternative hypothesis and this fact will lead us to decide which model we should prefer, taking into account that we do not want to reject incorrectly H_0 in more than $100(1-\alpha)$ % of the cases, where α is the chosen size of the test.

According to the standard theory of statistical tests we have to determine and compare the likelihood functions under H_0 and under H_1. We find for these functions the following analytic expressions:

$$L(H_0,\lambda,a:\vec{Q}=\vec{q}) = \left(\frac{\lambda}{a}\right)^{(2n-1)N} \prod_{l=1}^{N} \prod_{i=-(n-1)}^{n-1} \exp\left(-\frac{\lambda\, q^{(l)}(i/(2n))}{a}\right) ,$$

and

$$L(H_1,\lambda,a:\vec{Q}=\vec{q}) = \left(\frac{\lambda}{a}\right)^{(2n-1)N} \prod_{i=-(n-1)}^{n-1} \left[\left(\frac{1}{b(i/(2n))}\right)^{N} \times \prod_{l=1}^{N} \exp\left(-\frac{\lambda\, q^{(l)}(i/(2n))}{a\, b(i/(2n))}\right) \right] .$$

It is interesting to note that both likelihood functions depend on λ and on a only in terms of $\rho = \lambda/a$ whenever the values of $b(i/(2n))$ are not expressed in terms of a. If this condition is fulfilled only the parameter ρ is relevant, since a change of a (size factor) can be counterbalanced by a change of λ (factor of cross-sectional deformation). According to the fundamental theorem of Neyman-Pearson the recommended test statistic for testing H_0 versus H_1 takes for given ρ (and for given a in case A) the form

$$\Lambda^* = L(H_1,\rho:\vec{Q})/L(H_0,\rho:\vec{Q}) = \prod_{i=-(n-1)}^{n-1} b(i/(2n))^{-N} \times \exp\left[\rho \sum_{l=1}^{N} \sum_{i=-(n-1)}^{n-1} Q^{(l)}(i/(2n)) \left(1-\frac{1}{b(i/(2n))}\right)\right] .$$

The critical region of the optimal test is formed by the $100(1-\alpha)$% largest values of Λ^* under H_0. It is evident that Λ^* can be replaced by the equivalent test statistic

$$T_{N,n} = \rho \sum_{l=1}^{N} \sum_{i=-(n-1)}^{n-1} Q^{(l)}(i/(2n)) \left(1-\frac{1}{b(i/(2n))}\right) .$$

The test accepts the alternative shape-type if the value of $T_{N,n}$ is sufficently large.

Note that $Q^{(l)}(i/(2n))$ follows under H_0 an exponential distribution with parameter ρ and that this implies that $\rho Q^{(l)}(i/(2n))$ follows under H_0 a standard exponential distribution. Based on this consideration we find for the first and second moments under H_0 the expressions:

$$m_{N:n} := E[T_{N,n}:H_0] = N \sum_{i=-(n-1)}^{n-1} \left(1-\frac{1}{b(i/(2n))}\right) ,$$

and

$$v_{N:n} := \mathrm{Var}[T_{N,n}:H_0] = N \sum_{i=-(n-1)}^{n-1} \left(1-\frac{1}{b(i/(2n))}\right)^2 .$$

Since $T_{N,n}$ may be represented as the sum of N random variables,

$$T_{N,n}^{(l)} := \rho \sum_{i=-(n-1)}^{n-1} Q^{(l)}(i/(2n)) \left(1-\frac{1}{b(i/(2n))}\right), \quad [l=1,\ldots,N] ,$$

which are independent and identically distributed, $T_{N,n}$ is for fixed n and for $N \to \infty$ asymptotically normally distributed with mean $m_{N:n}$ and with variance $v_{N:n}$. This allows to determine the asymptotic critical value $c_{N:n}(1-\alpha)$ for the test of size α. We find $c_{N:n}(1-\alpha) = m_{N:n} + (v_{N:n})^{1/2} z(1-\alpha)$, where $z(1-\alpha)$ satisfies $\Phi(z(1-\alpha)) = 1-\alpha$ and is tabulated and Φ designates the distribution function of the standard normal distribution. The critical region of the test is thus given by $T_{N,n} > c_{N:n}(1-\alpha)$.

FURTHER INDICATIONS FOR PARTICULAR SHAPE ALTERNATIVES

In order to be able to implement the test the values $b(i/(2n))$ for $i = -(n-1), \ldots, n-1$ have to be known. In the cases A, B, C and D and for the planar and for the spatial version of the problem the following results are obtained by elementary calculations:

- Case A, planar particles:
  $b(i/(2n)) = \sqrt{1-i^2/n^2}/a$
- Case A, spatial particles:
  $b(i/(2n)) = \sqrt{1-i^2/n^2}/a$
- Case B, planar particles:
  $b(i/(2n)) = (4/\pi)\sqrt{1-i^2/n^2}$
- Case B, spatial particles:
  $b(i/(2n)) = (\sqrt{3/2})\sqrt{1-i^2/n^2}$
- Case C, planar particles:
  $b(i/(2n)) = (1-(1/n))$ or $1+(i/n)$
- Case C, spatial particles:
  $b(i/(2n)) = \sqrt{3}[(1/2)-(i/(2n))]$ or
  $\sqrt{3}[(1/2)+(i/(2n))]$.
- Case D, planar particles:
  $b(i/(2n)) = ((\sqrt{5}/4)+\ln((\sqrt{5}+1)/2))^{-1}$
  $\sqrt{1+i^2/(4n^2)}$
- Case D, spatial particles:
  $b(i/(2n)) = \sqrt{12/13}\sqrt{1+i^2/(4n^2)}$.

EXTENSION OF THE METHOD

The described method can also be applied to particles with axial symmetry which have for some straight-lines at some ordinate levels more than two intersection points with their boundary when we replace the measurement of the cross-sectional breadth by the measurement of the total (maximal) length of the segments of intersection between the particle and the lines $y = i/(2n)$ respectively $z = i/(2n)$. Since our random deformations do not change the number of these segments, choosing between shape types exhibiting a different number of segments at the same measurement level under H_0 and under H_1 is easy and leads to a clear-cut rejection of (at least) one of the hypotheses.

It is worthwhile to note that our procedure is not restricted to exponentially distributed dilatation factors; the method may be applied in an similar way if the deformation factors follow other distributions on $\mathscr{R}^+$ and even in the case of interdependence between the factors associated to the same particle.

RELATED WORK

The idea to interpret observed particles as randomly deformed prototypes is already expressed in the publications of Grenander (1993). In Hobolth *et al.* (2003) the sets are described by the normalized radius-vector function and its polar Fourier expansion. In Hobolth and Vedel Jensen (2000) the observed shape is a continuous stochastic deformation of a template curve by means of a zero mean stationary cyclic Gaussian process. In Kent *et al.* (2000) the observed figures are represented as deformed n-sided regular polygons. While these approaches work with transformed measurements to describe particles in general and lead thus to the necessity to find out which set of transformed measurements correspond to the shape-types to be distinguished, these shape-types are in my contribution introduced at the outset, since they are chosen as classes of admitted templates.

REFERENCES

Grenander U (1993). General pattern theory. Oxford:Oxford University Press.

Hobolth A, Pedersen J, Vedel Jensen EB (2003). A continuous parametric shape model. Ann Inst Statist Math 55(2):227–42.

Hobolth A, Vedel Jensen EB (2000). Modelling stochastic changes in curve shape, with an application to cancer diagnostics. Adv Appl Prob 32:344–62.

Kent JT, Dryden IL, Anderson CR (2000). Using circulant symmetry to model featureless objects. Biometrika 87(3):527–44.

Mukopadhyay N (2000). Probability and statistical inference. New York: M.Dekker, Ch. 8.

Stoyan D and Stoyan H (1992). Fraktale, Formen, Punktfelder. Methoden der Geometrie–Statistik. Berlin: Akademie Verlag, pp.81–2.

Streit F (1997). Sur des tests statistiques utiles pour la reconnaissance des formes. Archs Sci Genève 50:217-22.

Streit F (2000). Recognition of the type of figures by methods of statistical identification. Rendiconti del Circolo Matematico di Palermo, Ser. II, Suppl. 65:317-28.

Streit F (2003). On the choice of the stochastic model for random sets generated from angular density functions. In: Voinov V, ed. Advances in statistical inference methods: theory and applications. Almaty: Kimep, 443–6.

Streit F (2005). On the choice of copula in modelling dependence relations for random sets. In: Chrapoński J, Cwajna J, Wojnar L, eds. Proc 9th Eur Congress Stereol Image Analysis; 7th Int Conf Stereol Image Anal Mater Sci STERMAT. Zakopane: vol. II, 267–72.

Streit F (2006). On the multiplicative deformation model for random sets. Rendiconti del Circolo Matematico di Palermo, Ser. II, Suppl. 77:635–42.