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The Power of Parametric Orientation Statistics in the Earth Sciences

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With 6 figures and 1 table

Abstract

The problem of determining reliably the "mean" orientations contained in a series of clusters of axes is discussed. The correct parametric procedure, based on the determination of the eigenvectors of an orientation matrix, is recalled. The extension to more than one distribution is presented, and a new version for the determination of the preferred (one or more) directions of data on a circle is given. It is shown that parametric statistics is a powerful tool for determining such "means" from relatively few data (of the order of 10–30 data for 1 to 3 maxima).

Examples that demonstrate the power of these procedures are given.

Zusammenfassung

Die Effizienz der parametrischen Richtungsstatistik in den Erdwissenschaften.

Es wird das Problem der Bestimmung von representativen mittleren Achsen aus einer Serie von räumlichen Achsen erläutert. Dabei wird angenommen, daß die Achsen unter Umständen nicht deutlich erkennbare Häufungen (Clusters) aufweisen. Ausgehend von der exakten parametrischen Lösung für einen Häufungspunkt wird die Erweiterung zu mehreren sich überlagernden Häufungen dargestellt. Eine neue Methode zur Behandlung von Richtungen (Häufungen am Kreis) wird vorgestellt. Insbesondere wird gezeigt, daß mit parametrischen Methoden schon aus einer kleinen Zahl von Werten (nämlich ca. 10 bzw. ca. 30 Meßwerte für 1 bzw. 3 Achsen) die mittleren Orientierungen oder Richtungen mit angehörigem Vertrauensbereich gefunden werden. Die Vorteile dieser Methode werden an Hand von Beispielen aus der Natur erläutert. Die Rechenprogramme können, soweit sie von den Autoren selbst erstellt wurden, von diesen bezogen werden.

1. Introduction

In the Earth sciences, one is often faced with the problem of determining reliably the "mean" orientation embodied by one or several clusters of axes. These axes may refer to fault plane solutions of earthquakes, to joint planes, to grain orientations, to

the normals of bedding planes etc. Usually, the problem is solved graphically by plotting poles or such like on an equal-area projection of a unit sphere and drawing isolines by hand. The question, then, arises as to how many data are necessary for getting "reliable" results: Some structural geologists claim that thousands of measurements of the pertinent data have to be taken at each outcrop, others think that a few tens or hundreds may be sufficient.

It is the aim of the present paper to show that the above questions can be answered by the application of parametric statistics and the corresponding statistical tests (DUDLEY, PERKINS and GINE 1975, WATSON, 1970): One assumes that the data have a distribution which is described by a preassumed function with a number of unknown parameters. This assumption is not really satisfied, but in practice it can be fulfilled very closely in many cases. If this assumption holds, one can obtain statistically meaningful centers of distributions with a very small number of data. The justification for the *a priori* assumption of the distribution function can be inferred from the various central limit theorems which indicate that data which are the mean of many independent distributions (coming from different unknown causes) have a normal distribution in linear space. On a sphere such a central limit theorem does not exist but there is some experimental evidence (KOHLBECK & SCHEIDEGGER, 1977, WATSON, 1970) that the DIMROTH–WATSON distribution or the more general Bingham-Distribution (MARDIA, 1972) plays the same role on a sphere as does the normal distribution on a line. If we assume that there are several independent physical causes which result in a scatter of the data (e. g. joint directions in an outcrop) and if we assume that the deviations are randomly distributed, we can state that the total distribution will be a linear superposition of single distributions. This total distribution can be matched to the experimental data by varying the parameters. From these parameters an estimate for the unknown centers can be made. This method has been applied by KOHLBECK & SCHEIDEGGER (1977) for axial data on a sphere and has proved to be very successful. For linear data, similar considerations can be made. In this case we have the advantage that the following limit theorem exists (see eg. MARDIA, 1972): If X_i, $i = 1 \ldots . n$ are independent and identically distributed random variables in the range $-\pi \leqq X_i \leqq \pi$ with expectation values $E(x_i) = 0$, then the distribution of

$$S_n = (\Sigma\, x_i/\sqrt{n}) \bmod 2\pi$$

tends towards the wrapped normal distribution with the parameter σ. This limit theorem confirms our assumption that many circular data have distributions which can be approximated by the wrapped normal distribution, or by a sum of wrapped normal distributions with different means and parameters. In the case when there is only one cluster or concentration of points, the mean value can be obtained very quickly with a least squares procedure [SCHEIDEGGER (1963, 1965) for spherical data; FISHER (1953) for circular data]. If there are more than one concentration, the problem is somewhat complicated [KOHLBECK & SCHEIDEGGER (1977) for spherical data] and will be described in the following sections.

These various methods will now be reviewed; examples will be given to demonstrate their power in every case.

2. Solution of the basic parametric problem

The basic problem is: For a random cluster of directions, which is the best "mean"?

Two approaches have been successfully used in the geosciences:

(1) The spherical mean, which is defined by the vector $\vec{l}_o = (l_o, m_o, n_o)$

$$l_o = \sum_{i=1}^{N} l_i/R \qquad m_o = \sum_{i=1}^{N} m_i/R \qquad n_o = \sum_{i=1}^{N} n_i/R$$

$$R = [(\Sigma\, l_i)^2 + (\Sigma\, m_i)^2 + (\Sigma\, n_i)^2]^{1/2}$$

with l_i, m_i and n_i the direction cosines of the N orientation data. This mean has been used e. g. by FISHER (1953) in paleomagnetism studies and is best suited for directed data or vectors.

(2) The axis of the extremal moment of inertia, which is best suitable for axial data. This "quadratic" mean has first been introduced by SCHEIDEGGER (1963, 1965, FARA & SCHEIDEGGER, 1963) in connection with various problems in geophysics.

It has been found that many geological and geophysical data which are clustered around one point on a sphere, can be well described by a FISHER-distribution, whereas axial data which are districuted on a hemisphere very often can be described by a DIMROTH (1963) – WATSON (1966) function. These distributions have the following densities.

FISHER distribution:

$$g(\theta, \varphi)\, da = A \cdot \exp(k \cdot (\vec{l}_i \cdot \vec{l}_o))\, da$$
$$A = k/(4\pi \cdot \sinh k)$$

DIMROTH–WATSON distribution:

$$f(\theta, \varphi)\, da = A \cdot \exp(k^2 \cdot (\vec{l}_i \cdot \vec{l}_o)^2)\, da$$
$$A = 1/4\pi \int_0 \exp(k^2 t^2)\, dt)$$

with $\vec{l}_i(\theta, \varphi)$ the direction of the simple point and $\vec{l}_o(\theta_o, \varphi_o)$ the mean direction k the concentration factor and $da = \sin\theta d\theta d\varphi$ the area element. It can be shown that the maximum likelihood estimator of l_o yields the spherical mean in the case of a FISHER distribution and yields the axis of inertia in the case of a DIMROTH–WATSON-distribution. The FISHER-distribution and the DIMROTH-WATSON-distribution are closely related to each other: We introduce the angle α between the pole of the distribution l_o and the random variable l by

$$\cos\alpha = \vec{l}_o \cdot \vec{l}$$

and obtain:

$$g(\theta, \varphi)\, da = A_g \cdot \exp(k_g \cos\alpha)\, da$$
$$f(\theta, \varphi)\, da = A_f \exp(k_f^2 \cdot \cos^2\alpha)\, da$$

with the identity: $\cos^2\alpha = 1/2(1+\cos 2\alpha)$ the last expression can be written:

with

$$f(\theta, \varphi)\, da = \bar{A} \exp(\bar{k}_f^2 \cdot \cos 2\alpha)\, da$$
$$\bar{A} = A_f \exp(k_f^2/2) \text{ and } \bar{k}_f = k_f/\sqrt{2}$$

Thus, the DIMROTH–WATSON distribution has the same shape as the FISHER-distribution if the angles between pole of distribution and random variable are doubled. The parameter k is indicative of the sharpness of the distribution. For low angles cos α can be approximated by 1-(1/2) α^2 and both $g(\theta, \varphi)$ and $f(\theta, \varphi)$ tend to a normal distribution.

3. Extension to multiple distributions in space

3.1 Theory

The problem of finding the parameters characterizing the best fitting axis for a cluster of axes can be solved, in three dimensions, by finding the eigenvalues and eigenvectors of a symmetric 3×3 matrix, i. e., in essence, by solving a third-order equation.

In many instances, the data do not belong to a single cluster, but to several clusters. Therefore, an automatic procedure must be devised in which the density-distributions for the axes is the superposition of several basic DIMROTH–WATSON distributions, each of which is characterized by the direction of its central axis (two parameters), by its value of k and by its amplitude A. Thus, each distribution is characterized by 4 parameters; however, since the integral over all the distributions must be 1, we note that N distributions are jointly characterized by 4N-1 parameters.

The theory for the definition of the "best fitting" 4 N-1 parameters is the same as with one distribution: The parameters must be defined in such a fashion that the likelihood of finding the actually found data becomes a maximum. This is achieved by directly maximizing the likelihood function first by a Monte Carlo search and then finding the actual maximum by various approximation procedures. The present writers have developed a corresponding algorithm (KOHLBECK and SCHEIDEGGER, 1977) starting from particular computer programs available in soft-ware libraries (e. g. JAMES and ROOS, 1971).

The effort for the maximization of the likelihood function (and thus of the "best fitting parameters") is substantial, but it can be fully automatized. Confidence limits, dispersions and the weights of the component-distributions can also be determined. All this information, of course, is tied up with the assumption that the natural data are indeed generated by DIMROTH–WATSON distributions. This is a reasonable but to some extent arbitrary assumption.

A further remark refers to the number of measurements that are necessary to determine the "mean" axes of the distributions. In the geological literature one finds estimates from hundreds to thousands of individual orientations that are deemed necessary for the fixation of the mean direction. However, it is a well known fact that around 3 measurements suffice for the determination of each parameter; the acutal confidence limits come out of the statistical calculation. Thus, for a single axis (3 parameters), 9 measurements would be required, for two axes (7 parameters), 21 measurements, for 3 axes (11 parameters), 33 measurements. Taking more measurements will not improve the confidence limits significantly: Either the data are indicative of (one, two or more) DIMROTH–WATSON distributions, or they are not. In the former case relatively few measurements will fix the parameters, in the latter, no

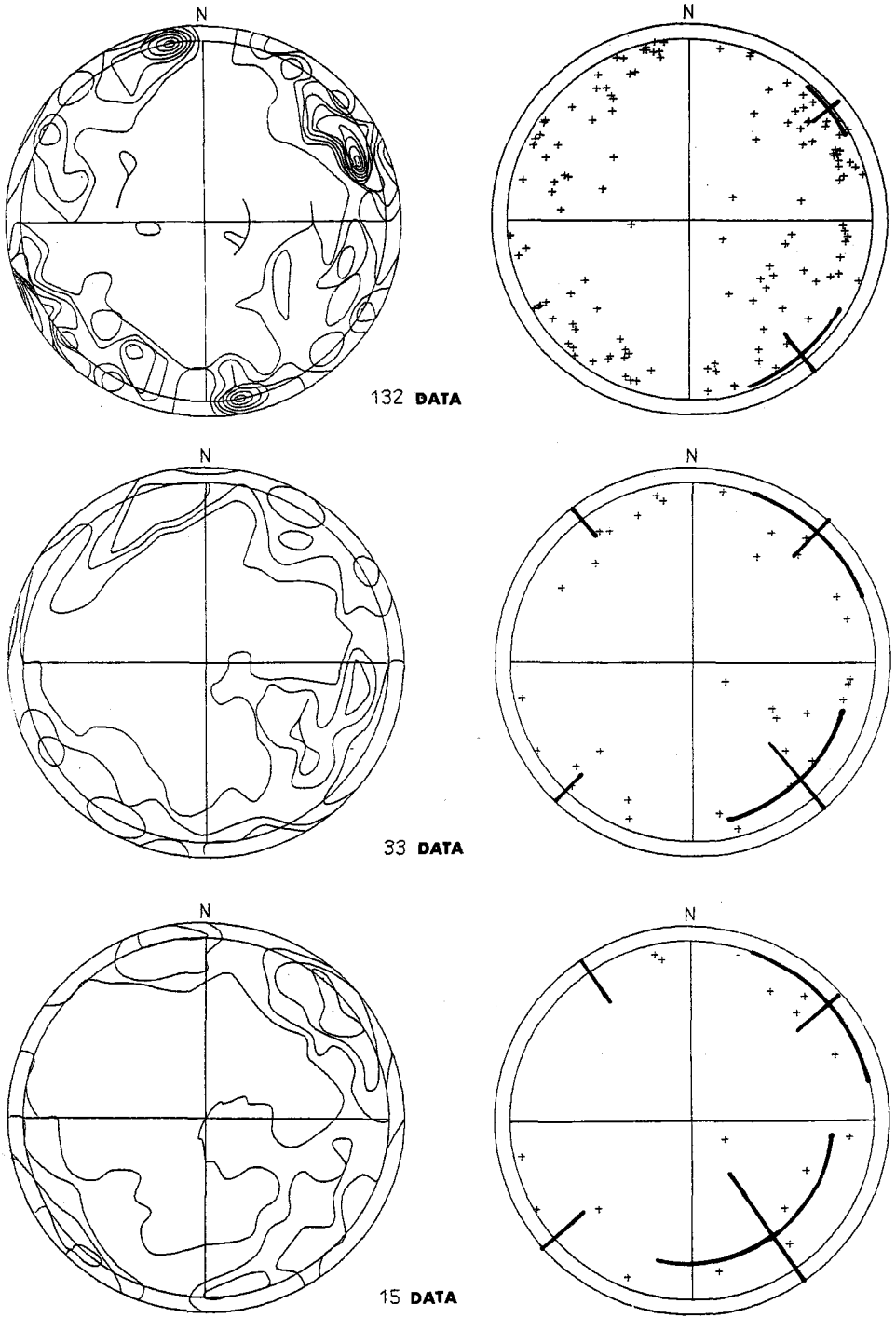

Fig. 1: Joint poles (right) and density lines (left) in equal area projection from one location with increasing number of data. Heavy line shows calculated error ranges of angle θ and φ of the centers of concentrations. (Ruetzstollen, Tyrol, Austria)

axes can be established with confidence regardless of the number of measurements taken.

3.2 Examples for the recognition of concentrations from samples of orientation data

The following examples show joint orientation measurements with poles of joints and density lines drawn on the lower hemisphere in equal area projection. The aim of these examples is to show that few data are sufficient to locate really existent concentrations with parametric statistics. Fig. 1 shows from bottom to top the poles and their densities with an increasing number of measurements embodying from 15 to 132 data. The heavy lines in the right pictures are the ranges of uncertainities for the angles ϑ and φ of the center obtained by the calculation with superposition of 2 DIMROTH–WATSON functions. It can be clearly seen that even in the case of 15 data points the centers are found very definitely. Increasing the number of data reduces the uncertainities, somewhat but the locations of the centers are not substantially changed. Fig. 2 shows a practical example where the distribution of joint poles is nearly random. No significant center could be found by calculations using up to 224 data points.

4. Circular distributions

4.1 Theory

We have seen that, on a sphere, the DIMROTH–WATSON distribution can be used for the approximation of actual densities in many cases. This is not the outcome of a limit theorem, but rather of a "correspondence principle" which shows that the DIMROTH–WATSON distribution approaches a Gaussian distribution if the sphere becomes very large, i. e. if it approaches a plane.

For circular data, one has the advantage that a limit theorem does actually exist (MARDIA, 1972). The latter states that, if X_i, $i = 1 \ldots n$ are independent and identically distributed random variables in the range $-\pi \leq X_i \leq \pi$ with expectation values $E(x_i) = 0$, then the distribution of

$$S_n = (\Sigma X_i/\sqrt{n}) \bmod 2\pi$$

tends towards the wrapped normal distribution with parameter $\sigma^2 = E(X^2)$.

This theorem is not directly applicable to the problem of the orientation of axes, because the latter only have a range

$$-\frac{\pi}{2} = X_i = \frac{\pi}{2},$$

but it can evidently be made applicable by a simple doubling of all the values of the variables, i. e. of the angles φ (that is: take $X_i = 2\varphi_i$). The method of doubling the angles has been used long ago by KRUMBEIN (1939) in connection with the study of the orientation statistics of sedimentological axes. Now the theory given above can be extended to distributions with several maxima in the density function, by simple superposition of wrapped normal distributions with different means and parameters.

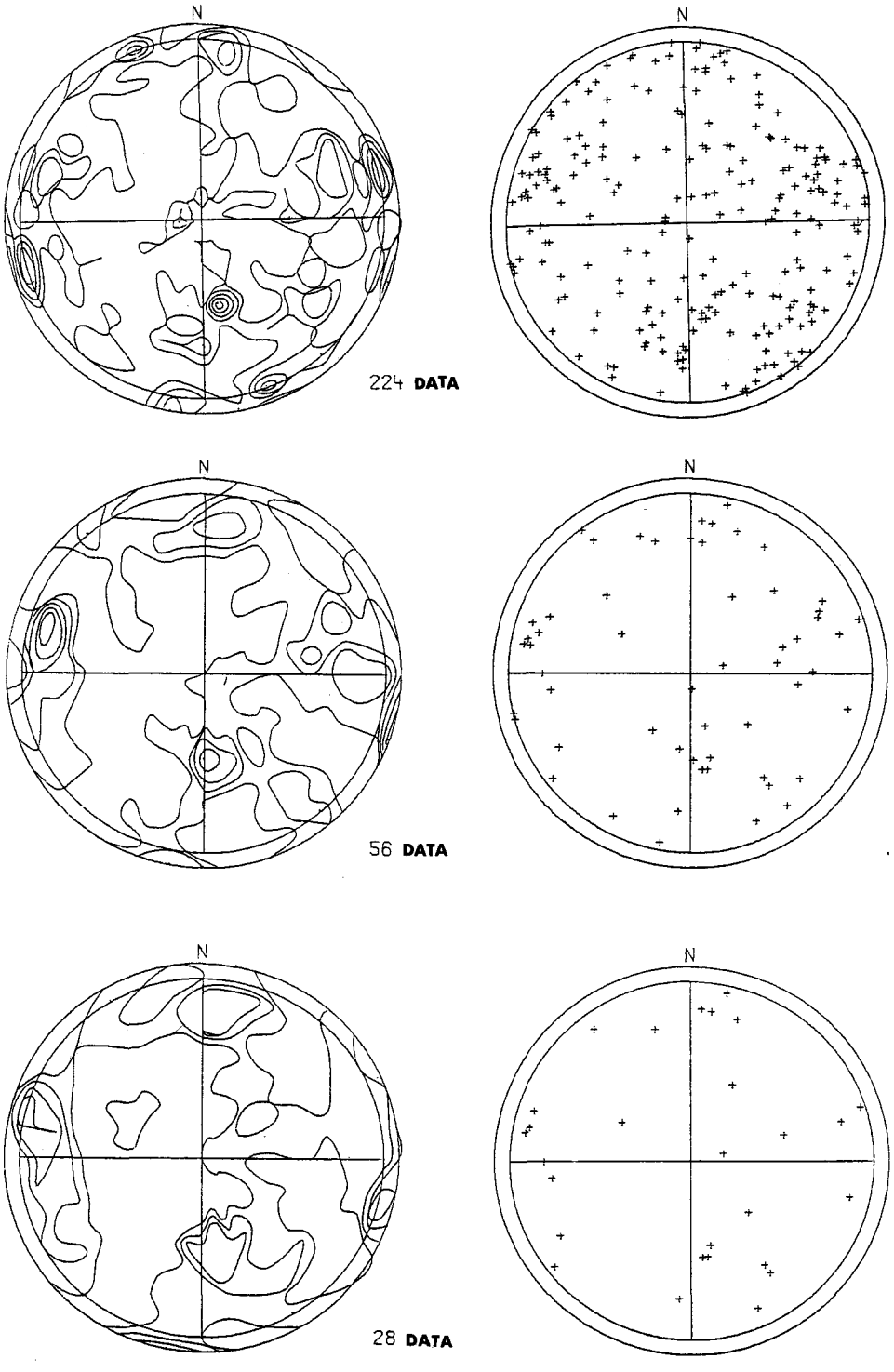

Fig. 2: Joint poles (right) and density lines (left) in equal area projection from one location with increasing number of data. (Salzburg near Hallstatt, Upper Austria)

Thus we assume that the probability density function of the data under consideration can be approximated by:

$$g(x)dx = \sum_{i=1}^{r} p_i f_i(x)\, dy \qquad 1 \leq r \leq 4$$

$$f_i(x) = \frac{1}{\sigma_i \sqrt{2\pi}} \sum_{k=-\infty}^{+\infty} \exp\left[(-1/2)\frac{(x - a_i + 2\pi k)^2}{\sigma_i^2}\right]$$

$$p_i > 0 \qquad \text{and} \qquad \sum_{i=1}^{r} p_i = 1$$

where the p_i are the weights of the wrapped normal distributions f_i with centers at a_i. The function g is fitted to N experimental data by minimization of the negative likelihood function

$$L\,(x/\underline{\theta}) = -\sum_{i=1}^{N} \ln g\,(x_i/\underline{\theta})$$

with respect to the n parameters

$$\theta = a_1, a_2 \ldots a_r; \sigma_1, \ldots \sigma_r; q_1, \ldots q_{r-1}$$

with

$$p_i = (1-q_{i-1}) \prod_{j=1}^{r-1} q_j$$

$$p_r = 1-q_{r-1}$$
$$q_o = 0$$

With the same arguments as those used by KOHLBECK and SCHEIDEGGER (1977) one obtains estimates for the errors of the parameters $\underline{\theta}$ found: if $\underline{\theta}$ is the likelihood estimator found and $\underline{\theta}_o$ some other estimated value of $\underline{\theta}$ and if we define

$$s = 2\,[L\,(x, \hat{\underline{\theta}}) - L\,(x, \underline{\theta}_o)]$$

then we have for the probability estimate:

$$p_r\,(s > \varsigma_\alpha) \approx \chi_n^2\,(\alpha)$$

where $\chi_n^2\,(\alpha)$ denotes the chi-square distribution with a degrees of freedom and significance-level α.

For the construction of the algorithm we used again a function-extremization program available in the software library (e. g. JAMES and ROOS, 1971). In each case, the validity of the solution must be checked as follows.

1st The values p_i must be considered. If the weight p_r of a function f_r is high and considerably greater than its error, this f_r will represent a real existing event. If p_r

is low or lower than its error, the maximum will most probably be spurios and only represent a disturbing or accidental event.

2nd The value of parameter σ must be considered. If σ is greater than about 30°, the function f_r represents most probably a diffuse background which is not caused by a special event. If σ is very sharp (less than 2° or 3°) only 1 or 2 data points are associated with f_r and f_r therefore is not representative. This happens if g contains more functions f_r than are necessary. The negative likelihood is somewhat lower in this case than in the case where the weight is set to zero.

3rd Applying points 1 and 2 one can eliminate the suspect maxima of the function g, and in some cases g will reduce to a case with a lower number r of functions f. If one considers all functions g with different r, the solution g with lowest negative likelihood function L will normally be the best.

4th The means of the functions f must be considered. If the errors are too high, the numbers of data are not high enough to fix the centers. In this case only the use of more data can ensure the solutions.

The outlined method can be used to locate the density functions for stochastically distributed circular data. The parameters can be found without plotting histograms of the data, but a visual check is very helpful in some cases. With respect to the usual, more intuitive interpretation of the data by the inspection of histograms, the method has the following advantages: Narrow distributions can be separated which hardly could be separated visually. The maxima can be located very accurately and approximate errors for their location can be stated. It has been found from a great number of evaluations of field data that far fewer experimental data are necessary for finding the centers with the same accuracy than are necessary with conventional methods.

4.2 Demonstration of the resolving power for circular data

In the following examples it is shown how far it is possible to recognize two adjacent clusters as separate ones. In the "cases" I to III below the input data are chosen to follow the truncated normal distribution. The density of this function goes to zero outside a limit value and therefore differs remarkably form the approximated wrapped normal in this range. "Case" IV represents really measured data.

Case I Superposition of 2 truncated normal distributions. The distribution functions go to zero at a distance of more than 16° from the mean and follow a normal distribution N (a, 1) in the range of 16° around the mean at a. The centers are located at 0° and 40° respectively as seen in fig. 3. The non-zero values of each distribution are well separated from each other.

Case II Same case as I, but the truncation is at 40° from the mean. The distribution functions are overlapping as seen in fig. 4.

Case III Same case as II, but the means are at distances 0° and 20°. The distributions are strongly overlapping and the greatest value of the common distribution occurs at 10°. (Fig. 5)

Case IV The distribution of valleys of Switzerland is drawn in the rose diagram of fig. 6.

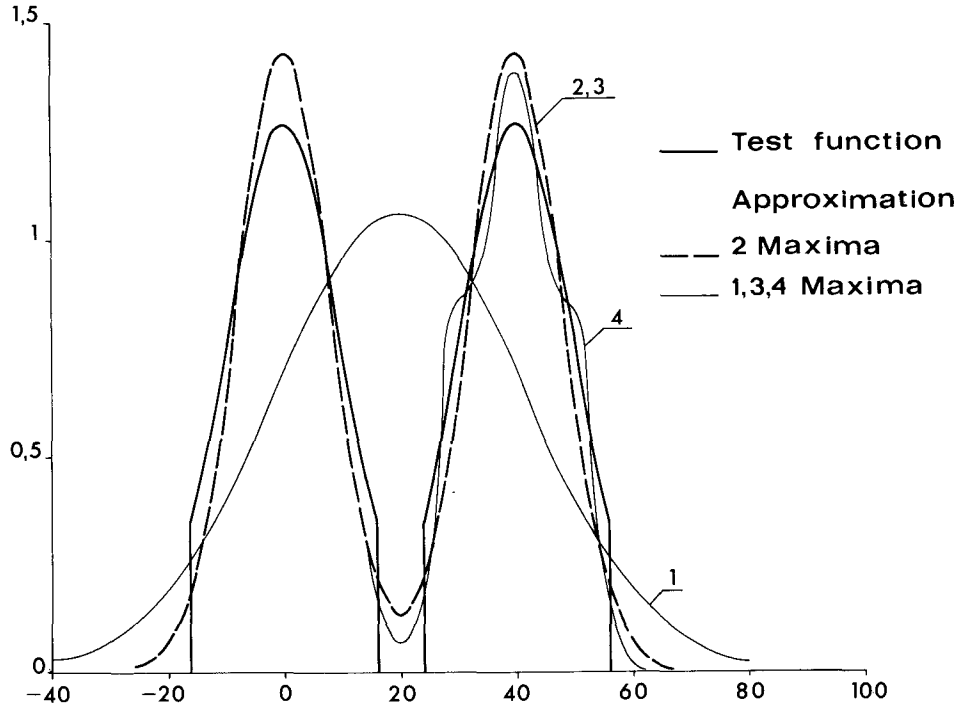

Fig. 3: Test function truncated normal and approximation by g(x) with number of maxima r = 1, 2, 3, 4. Function with r = 2,3 are identical and give best approximation.

Calculations are carried out by fitting the function g defined in (1) with superposition of 1, 2, 3 and 4 wrapped normals to each of the cases I, II, III. Figures 3 to 6 show the distribution functions y (x) of the input data and their approximations by g (x). Table 1 shows the calculated parameters p_i, a_i and σ_i of g with their estimated errors at the significance level of 0.3 and the value of the negative maximum-likelihood L.

Case I: The single distribution functions are well separated from each other. The correct solutions are found with r = 2 and r = 3, but the best value of L is found with r = 4. r = 4 shows the two correct maxima at 0° and 40° with great weight and two extra maxima with spurious weights at 51° and 29°. These weights with p_i = 0.07 and 0.08 are not remarkably greater than the errors. The maxima have σ = 3° and are on the limit of being acceptable. Comparison with the solution of r = 2 shows that the errors are greater with r = 4. However because L = 896 is lower than L = 1019 obtained with r = 2 no absolute decision could be made whether or not 4 maxima are correct, if the distribution function is not a priori known.

Case II: The distribution functions are overlapping. The solutions with r = 1 show again a diffuse background with the highest value of L. All other

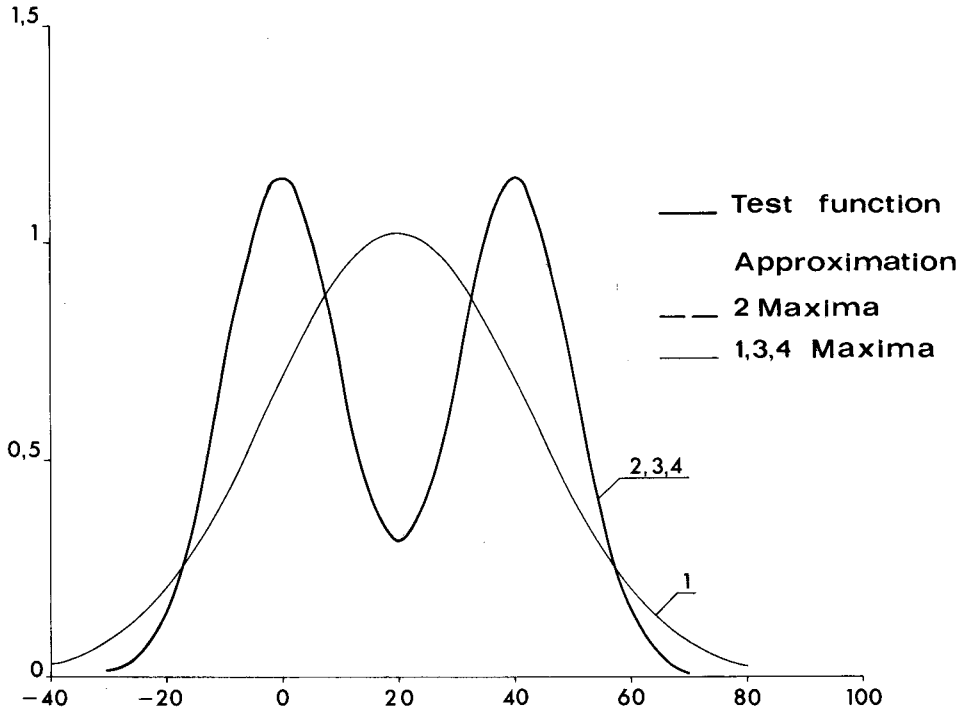

Fig. 4: Test function consists of a superposition of two overlapping normal distributions with well separated maxima. The approximation with g(x) and r = 2, 3, 4 gives nearly identical distributions.

solutions have about the same value of L and one can assume that the solution with the lowest r, that is with r = 2, is the best one. This is confirmed as follows. The solution with r = 2 shows two maxima with great weights and low errors. The solution with r = 3 has one maximum at a = 180° which is identical to that at a = 0 if r = 2. The weight of f corresponding to this maximum is 0.5 as is the case with r = 2, but the error is 0.45 which is at the limit of being acceptable. The errors of the two other maxima in weight are greater than the weights. Therefore this solution cannot be accepted. Similar considerations hold for r = 4.

Case III: The single distribution functions are strongly overlapping. The total density shows the greatest value between the means of the single functions f. If one tries g with r = 2 all parameters are found with their correct values (see table 1). If one takes r = 3 one obtains one function f with vanishing p. The remaining two functions f are similar to the expected ones, but not quite correct. The means differ by 4° and the weights have the ratio 1 : 2 instead of 1 : 1. The likelihood-function L (L = 36) is appreciately higher than that with r = 2 (L = 27).

The approximation with r = 1 and r = 4 gives 1 maximum located at

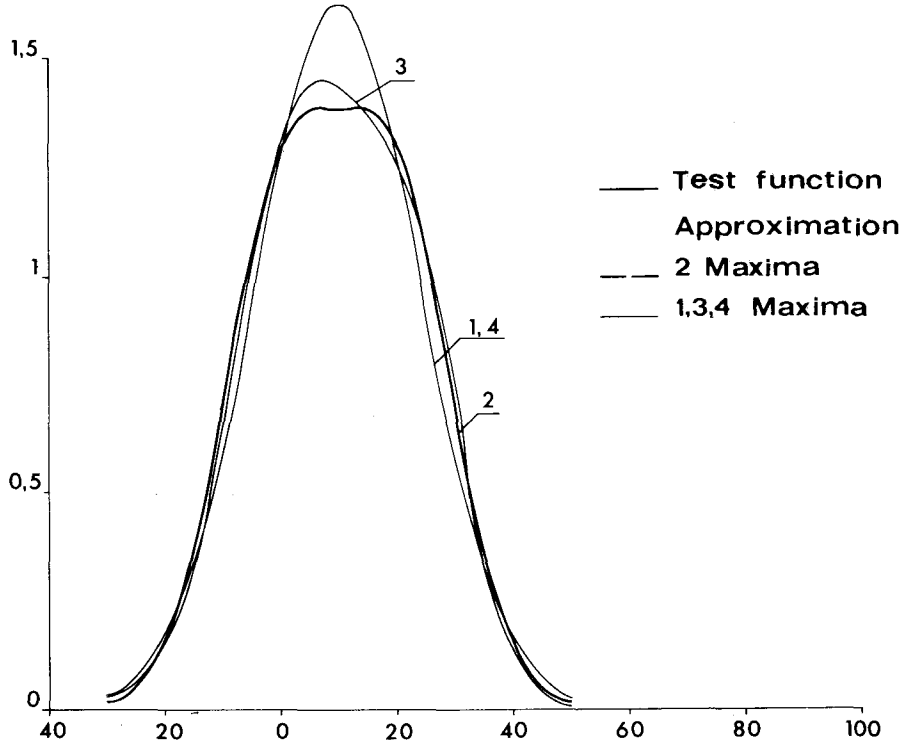

Fig. 5: Test function consists of a superposition of two strongly overlapping normal distributions with centers at 0 deg. and 20 deg. Both maxima are resolved by g(x) with r = 2. Within the usual limits of error this function can also be approximated with r = 1, 3, 4 but fit is somewhat poorer in this case.

10° which is the middle of the two really existing maxima. The likelihood-function gives L = 123 and indicates that the solution is by far the worst one. Therefore a consideration of the output-parameters shows clearly that the right solution is that with 2 maxima, which is completely in conformity with the input distribution.

Case IV: Example with field data (Fig. 6)
All solutions with r = 1 show two maxima at about 150° and 60° with highest weights. The ratio of weights to errors is by far the best for r = 2. L is about the same for all solutions. Therefore, there is no doubt that the solution with r = 2 is the best and the centers of the single distributions are at a = 145° and a = 56°.

5. Conclusions

It has been seen that the application of parametric methods can be advantageously used to locate density maxima: The parameters can be found without plotting histograms of the data, but a visual check is very helpful in some cases. Close

Table 1: Parameter values obtained by fitting the function $g(x) = \sum_{i=1}^{r} p_i f_i(x)$ to the funtions of case I to case IV. Given are the values and their errors at significance level 0.3 separated by /.

case	Parameter	unit	r = 1	r = 2		r = 3			r = 4			
			f_1	f_1	f_2	f_1	f_2	f_3	f_1	f_2	f_3	f_4
I	a	Degrees	20.0/.5	.0/.4	40.0/.4	40.0/.5	.0/.5	–	40.1/2.9	51.2/2.7	29.1/2.8	.1/.5
	σ	Degrees	21.5/.3	8.0/.2	8.0/.2	8.0/.3	8.0/.3	–	5.8/.9	2.9/1.3	3.0/1.3	8.0/.3
	p	–	1.00/0.00	.50/.02	.50/.02	.50/.02	.50/.02	–	.35/.09	.07/.06	.08/.07	.50/.02
II	a	Degrees	20.0/.5	40.0/.6	.0/.6	42.8/8.2	179.9/.7	35.9/3.9	40.8/3.5	7.6/9.5	178.3/3.6	27.4/49.4
	σ	Degrees	22.3/.3	9.9/.4	9.9/.4	9.2/1.7	9.9/.4	9.7/3.4	9.6/1.1	6.7/5.6	9.3/1.2	11.8/18.0
	p	–	1.00/0.00	.50/.02	.50/.02	.29/.34	.50/.46	.21/.60	.45/.42	0.06/.14	.42/.37	.06/.81
III	a	Degrees	10.0/.3	20.0/2.9	180.0/2.9	23.6/2.2	4.0/1.5	–	10.0/.5	–	–	–
	σ	Degrees	14.1/.2	9.8/.9	9.8/.9	8.7/1.0	11.5/.5	–	14.1/.3	–	–	–
	p	–	1.00/0.00	.50/.14	.50/.14	.31/.09	.69/.09	–	1.00/0.6	–	–	–
IV	a	Degrees	–	145.0/8.1	56.3/5.6	55.5/7.2	151.2/8.3	108.7/4.8	36.7/3.3	154.0/29.5	65.6/3.4	112.0/23.6
	σ	Degrees	–	35.5/12.9	20.2/7.0	23.2/8.4	24.0/9.6	6.1/2.8	4.9/2.1	35.7/15.7	10.1/2.7	17.1/16.2
	p	–	–	.60/.19	.40/.19	.49/.15	.43/.15	.08/.06	.10/.13	.57/.51	.26/.26	.08/.78

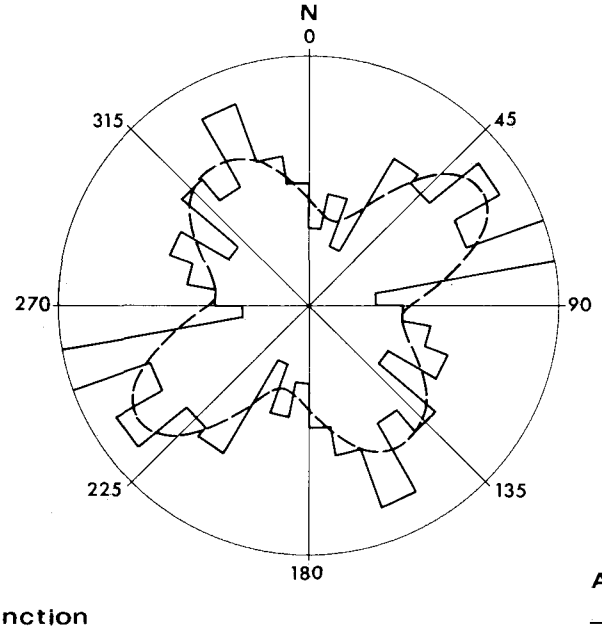

Fig. 6: Typical field example and approximation by g(x) with r = 2 drawn in a rose diagram: Weighted valley directions of Switzerland.

distributions can be separated which hardly could be separated visually. The maxima can be located very accurately and approximate errors for their location can be stated. It has been found from a great number of evaluations of field data that far fewer experimental data are necessary for finding the centers with the same accuracy than are necessary with conventional methods.

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