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DISTRIBUTION OF DIRECTIONAL DATA AND FABRIC TENSORS

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Abstract—Distribution of directional data is characterized by what is termed fabric tensors. A formal least square approximation is applied, and three kinds of fabric tensors are defined in connection with the choice of a basis of the space of functions on a unit sphere or a unit circle. All the resulting equations are Cartesian tensor equations, and they are interpreted in terms of the representation theory of the rotation group and the potential theory in electrodynamics. It is also shown how this characterization is related to the spherical harmonics expansion or the Fourier series expansion. Finally, a method of statistical test is presented in the Cartesian tensor form to check the true form of the distribution. A physical example is also given to illustrate the proposed technique.

1. INTRODUCTION

PHYSICAL and engineering systems involve not only scalar quantities but also vector and tensor quantities. Therefore, many experiments require measurement of orientations, e.g. orientations of velocity, polarization, or magnetization, principal axes of stress or strain, crystallographic axes, etc. Orientation of a surface is characterized by the direction of its normal vector, so that directional data also arise in observation of interfaces or crack surfaces in a material. After obtaining these directional data, we must interpret them in terms of given external control factors. A typical example is the study of the mechanics of granular materials from the microscopic viewpoint, where the material is idealized as an assembly of solid spheres or circular plates. There, a considerable achievement has been made in regard to techniques of observing the distribution of interparticle contact directions and theories of interpreting it in terms of the external loading [1–12].

The statistics of directional data is an old subject, perhaps dating back to Gauss, Bernoulli, Rayleigh, von Mises and the like, and the modern statistical approach was initiated by people like Pearson, Fisher and Rao, to name a few. (For details, see Mardia[13].) However, these people have devoted themselves mainly to non-physical problems such as geography, biology, ecology and social study. If, on the other hand, the underlying problem is a physical one, any description of physical laws must be expressed in the frame indifferent form, i.e. tensor equations invariant to coordinate transformations[14, 15]. It seems, however, that existing theories on the statistics of directional data are lacking this point of view, or at least only small attention has been paid to it so far.

In the following, the term "direction" or "orientation" actually means "axis", and the direction indicated by a unit vector $\boldsymbol{n}$ is identified with that indicated by $-\boldsymbol{n}$. Extension to the analysis of "truly directional" data is very easy. We first apply the least square approximation and define three kinds of "fabric tensors" in connection with the choice of a basis of the space of functions on a unit sphere or a unit circle. All the resulting equations are Cartesian tensor equations, and they are interpreted in terms of the representation theory of the rotation group and the potential theory in electrodynamics. We also examine the relationship to the spherical harmonics expansion and the Fourier series expansion. This consideration leads to many useful formulae of computing necessary quantities and converting one form into another. Finally, we present a method of testing whether observed data are regarded as a sample from a given distribution, applying the asymptotic statistical theory of testing the fitness of distribution by the use of the "Fisher information matrix". This is also obtained in the form of Cartesian tensor equations. Both two and three dimensional cases are analyzed.

As an illustrating example, we analyze the data of interparticle contact distribution of a two dimensional granular material observed by Konishi *et al.*[16] to demonstrate our technique. However, application of this theory is not limited to the mechanics of granular materials. It can be applied to a wide variety of physical, mechanical and geological problems. Moreover, it can be combined with the so called "stereological principles" to detect the structural anisotropy from observed data on a random cross section. Our formulation gives a practical procedure expressed in Cartesian tensor equations[17].

2. APPROXIMATION OF DISTRIBUTION AND FABRIC TENSORS

Let $\boldsymbol{n}^{(1)}$, $\boldsymbol{n}^{(2)}, \ldots$ and $\boldsymbol{n}^{(N)}$ be observed directional data, where each member is a unit vector. The most fundamental quantities are various averages of them. Since we are trying to seek tensor quantities to characterize the data distribution, we first consider the average of their tensor product, or the "moment", and put

$$N_{i_1 i_2 \ldots i_n} = \langle n_{i_1} n_{i_2} \ldots n_{i_n} \rangle, \tag{2.1}$$

where $\langle\,\rangle$ designates the sample mean, e.g. $\langle n_i n_j \rangle = \sum_{\alpha=1}^{N} n_i^{(\alpha)} n_j^{(\alpha)}/N$. We term $N_{i_1 \ldots i_n}$ the "moment tensor" or the "fabric tensor of the first kind" of rank n. This is a symmetric tensor, and any contraction of it lowers the rank, e.g. $N_{ijklmm} = N_{ijkl}$, etc. due to $n_i n_i = 1$. (Throughout this paper, we adopt the summation convention over tensor indices). This tensor plays a fundamental role in deriving tensor quantities characterizing the sample distribution, for all relevant information is contained in this tensor. However, it is not easy to understand the intuitive meaning of this tensor, and hence we now try to derive various characteristics in connection with the form of the "distribution density" of $\boldsymbol{n}$. Let $f(\boldsymbol{n})$ be the "empirical" distribution density, namely

$$f(\boldsymbol{n}) = \frac{1}{N} \sum_{\alpha=1}^{N} \delta(\boldsymbol{n} - \boldsymbol{n}^{(\alpha)}). \tag{2.2}$$

In the three dimensional case, $\delta(\boldsymbol{n} - \boldsymbol{n}^{(\alpha)}) = \delta(\theta - \theta^{(\alpha)})\delta(\phi - \phi^{(\alpha)})/\sin\theta^{(\alpha)}$, where $\delta(.)$ is the Dirac delta function, and θ and ϕ denote the spherical coordinates of $\boldsymbol{n}$, i.e. $\boldsymbol{n}^{(\alpha)} = (\sin\theta^{(\alpha)} \cos\theta^{(\alpha)}, \sin\theta^{(\alpha)} \sin\theta^{(\alpha)}, \cos\theta^{(\alpha)})$. In the two dimensional case, $\delta(\boldsymbol{n} - \boldsymbol{n}^{(\alpha)}) = \delta(\theta - \theta^{(\alpha)})$, where θ is the polar coordinate of $\boldsymbol{n}$, i.e. $\boldsymbol{n}^{(\alpha)} = (\cos\theta^{(\alpha)}, \sin\theta^{(\alpha)})$. Then, it is easy to see

$$\int f(\boldsymbol{n})\,\mathrm{d}\boldsymbol{n} = 1, \quad \int n_{i_1} \ldots n_{i_n} f(\boldsymbol{n})\,\mathrm{d}\boldsymbol{n} = \langle n_{i_1} \ldots n_{i_n} \rangle, \tag{2.3}$$

where $\mathrm{d}\boldsymbol{n}$ is the differential solid angle, i.e. $\int \mathrm{d}\boldsymbol{n} = \int_0^{\pi} \int_0^{2\pi} \sin\theta\,\mathrm{d}\phi\,\mathrm{d}\theta$ in the three dimensional case and $\int \mathrm{d}\boldsymbol{n} = \int_0^{2\pi} \mathrm{d}\theta$ in the two dimensional case. In general, $\langle . \rangle = \int (.) f(\boldsymbol{n})\,\mathrm{d}\boldsymbol{n}$. However, $f(\boldsymbol{n})$ is a very singular function. Hence, we now try to approximate the empirical distribution density $f(\boldsymbol{n})$ by a smooth one. This problem of smoothing is also viewed as a problem of estimating the "true" population distribution.

In general, the estimation of distribution is achieved by first assuming a "model" or a "parametric form", i.e. a family of distributions involving several parameters and second introducing some form of "measure of approximation" or the "distance" between two distributions. Then, the parameters are chosen in such a way that the introduced measure of approximation is maximized or the distance is minimized. Let $f(\boldsymbol{n})$ be a given distribution density, and consider a problem of approximating it by $F(\boldsymbol{n})$ which involves indeterminate parameters. Typical parametric forms of $F(\boldsymbol{n})$ are:

(I) $$F(\boldsymbol{n}) = C + C_i n_i + C_{ij} n_i n_j + C_{ijk} n_i n_j n_k + \cdots, \tag{2.4}$$

(II) $$F(\boldsymbol{n}) = [C + C_i n_i + C_{ij} n_i n_j + C_{ijk} n_i n_j n_k + \cdots]^2, \tag{2.5}$$

(III) $$F(\boldsymbol{n}) = \exp[C + C_i n_i + C_{ij} n_i n_j + C_{ijk} n_i n_j n_k + \cdots]. \tag{2.6}$$

Equation (2.4) is a polynomial in $\boldsymbol{n}$ and hence is easy to handle. However, the coefficients must be chosen so that $F(\boldsymbol{n})$ does not become negative. Equation (2.5) is always non-negative, and eqn (2.6) is always positive. The form of eqn (2.6) is sometimes referred to as the "exponential family"[18], [19] and is an extension of the "von Mises distribution" in the two dimensional case and the "Fisher distribution" in the three dimensional case (see[13]).

Meanwhile, typical criteria of approximation are:

(I′)
$$\int [F(\boldsymbol{n}) - f(\boldsymbol{n})]^2 \, d\boldsymbol{n} \to \min, \tag{2.7}$$

(II′)
$$\int [\sqrt{F(\boldsymbol{n})} - \sqrt{f(\boldsymbol{n})}]^2 \, d\boldsymbol{n} \to \min, \tag{2.8}$$

(III′)
$$-\int f(\boldsymbol{n}) \log \frac{f(\boldsymbol{n})}{F(\boldsymbol{n})} \, d\boldsymbol{n} \to \max. \tag{2.9}$$

All of these are applied on the condition that $\int F(\boldsymbol{n})\, d\boldsymbol{n} = 1$. Criterion (I′) is the "least square error approximation", or the approximation in L^2 on S^2 (a unit sphere) or on S^1 (a unit circle). This can be applied if $f(\boldsymbol{n})$ is the empirical density of eqn (2.2) because (I′) is equivalent to $\int F(\boldsymbol{n}) f(\boldsymbol{n})\, d\boldsymbol{n} \to$ max., and eqn (2.2) is an integrable function over S^2 or S^1. The measure of (II′) is sometimes referred to as the "Hellinger distance". However, it cannot be applied to the empirical density of eqn (2.2) because its square root is not defined. The measure of (III′) is the "entropy"[7] or the "Kullback information"[20]. It is derived as the logarithm of the probability that the empirical distribution $f(\boldsymbol{n})$ is observed when the true population distribution is $F(\boldsymbol{n})$ in the limit of an infinite number of samples. It can be applied if $f(\boldsymbol{n})$ is the empirical density of eqn (2.2) because (III′) is equivalent to $\int f(\boldsymbol{n}) \log F(\boldsymbol{n})\, d\boldsymbol{n} \to$ max., which yields the "maximum likelihood estimation". Both the measure of (II′) and the square root of the measure of (I′) give true "distances", satisfying the triangular inequality and being symmetric, while that of (III′) is only a "quasi-distance".

All these measures are invariant to coordinate rotations and hence have invariant meanings. In the case of "linear" distributions, i.e. in the case of non-directional scalar data, only (II′) and (III′) are invariant to transformations of the coordinate system. As we can see in the following, the mathematical structure for distributions of directional data is very much different from those of linear distributions, due to the fact that a distribution density of directional data is a function on S^2 or S^1, both of which is a topologically "compact" space.

Many other parametric forms and measures of approximation are possible, and any combination of a parametric form and a measure of approximation could be adopted for parameter estimation. In this paper, however, we consider only (I) and (I′). This is because this pair alone derives characteristics of distributions in terms of linear expressions of $N_{i_1 \ldots i_n}$'s. All necessary quantities are explicitly determined by linear calculations. Instead, of course, approximated distributions could be negative theoretically. However, this does not happen for most of practical problems. Moreover, our aim is not to describe distributions accurately but rather to characterize them by tensors, which are then related to macroscopic physical quantities. If the form of distribution itself is our aim, then other forms and measures must be employed at the cost of simplicity.

As we see later, the least square approximation of the polynomial expansion turns out nothing but the spherical harmonics expansion in the three dimensdional case and the Fourier series expansion in the two dimensional case. Thus, the use of spherical coordinates or polar coordinates would make the formulation much more familiar to us. However, our purpose is to derive tensor characteristics, which we generally term "fabric tensors", invariant to coordinate transformations, and hence we try to derive useful formulae and schemes of statistical testing in Cartesian tensor equations.

3. FABRIC TENSORS OF THE SECOND KIND

We first consider the three dimensional case. We assume that for each orientation a pair of unit vectors with opposite directions are to be generated so that $f(\boldsymbol{n})$ is a symmetric function with respect to the origin. (The case of non-symmetric distribution is discussed later.) Combining (I) and (I′) of the previous section, let us consider the following scheme:

$$E = \int [(C + C_{ij}n_i n_j + C_{ijkl}n_i n_j n_k n_l + \cdots) - f(\boldsymbol{n})]^2 \, d\boldsymbol{n} \to \min. \tag{3.1}$$

Terms of odd powers of $\boldsymbol{n}$ need not be included, since $f(\boldsymbol{n})$ is symmetric. However, it is easy to see that the coefficients are not uniquely determined. This is because 1, n_in_j, $n_in_jn_kn_l$ ... are not linearly independent. In fact, contraction of n_in_j over $i=j$ yields 1, contraction of $n_in_jn_kn_l$ over $k=l$ yields n_in_j and so on. Let V_n be the vector space of functions on S^2 spanned by $n_{i_1}\dots n_{i_n}$'s. In view of the symmetry, its dimension is $(n+1)(n+2)/2$. What we have observed is that $V_0\subset V_2\subset V_4\subset\dots$. Hence, if we want approximation up to the nth order, $n_{i_1}\dots n_{i_n}$ alone is sufficient as a basis. This means that it is sufficient to assume the nth approximation in the form

$$f(\boldsymbol{n})\sim\frac{1}{4\pi}F_{i_1\dots i_n}n_{i_1}\dots n_{i_n}, \tag{3.2}$$

from the beginning. We call the coefficient tensor $F_{i_1\dots i_n}$ the "fabric tensor of the second kind" of rank n. It is determined by $\partial E/\partial F_{i_1\dots i_n}=0$, where E is the square error of the form of eqn (3.1). The equation becomes

$$F_{j_1\dots j_n}\overline{n_{j_1}\dots n_{j_n}n_{i_1}\dots n_{i_n}}=N_{i_1\dots i_n}, \tag{3.3}$$

where we have put $\overline{\,.\,}=\int(.)\,\mathrm{d}\boldsymbol{n}/4\pi$. Making use of identity

$$\overline{n_{i_1}n_{i_2}\dots n_{i_{2n}}}=\frac{1}{2n+1}\delta_{(i_1i_2}\delta_{i_3i_4}\dots\delta_{i_{2n-1}i_{2n})}, \tag{3.4}$$

where δ_{ij} is the Kronecker delta and ( ) designates the symmetrization of the indices, and taking successive contraction of eqn (3.3), we can determine all components of $F_{i_1\dots i_n}$. It takes on the form

$$F_{i_1\dots i_n}=\frac{2n+1}{2^n}\binom{2n}{n}[N_{i_1\dots i_n}+a^n_{n-2}\delta_{(i_1i_2}N_{i_3\dots i_n)}+a^n_{n-4}\delta_{(i_1i_2}\delta_{i_3i_4}N_{i_5\dots i_n)}+\dots+a^n_0\delta_{(i_1i_2}\delta_{i_3i_4}\dots\delta_{i_{n-1}i_n)}]. \tag{3.5}$$

An explicit expression for a^n_m is given in the next section.

Example 3.1

$$F=1, \tag{3.6}$$

$$F_{ij}=\frac{15}{2}\left[N_{ij}-\frac{1}{5}\delta_{ij}\right], \tag{3.7}$$

$$F_{ijkl}=\frac{315}{8}\left[N_{ijkl}-\frac{2}{3}\delta_{(ij}N_{kl)}+\frac{1}{21}\delta_{(ij}\delta_{kl)}\right], \tag{3.8}$$

$$F_{ijklmn}=\frac{3003}{16}\left[N_{ijklmn}-\frac{15}{13}\delta_{(ij}N_{klmn)}+\frac{45}{143}\delta_{(ij}\delta_{kl}N_{mn)}-\frac{5}{429}\delta_{(ij}\delta_{kl}\delta_{mn)}\right]. \tag{3.9}$$

Expression (3.2) in terms of $F_{i_1\dots i_n}$ has a compact form, and the number of tensor components necessary to compute is minimum. However, this approximation is inflexible. For example, suppose we want the $(n+2)$th approximation. Then, we must recompute the tensor all the way from the beginning. Is it not possible that the tensor is decomposed into several parts in such a way that some still have sense in higher approximations? This is exactly the problem of decomposing $n_{i_1}\dots n_{i_n}$'s into several meaningful groups. This is done as follows.

Since $V_0\subset V_2\subset V_4\subset\dots$, as we have observed, let $W_0=V_0$ and let W_n $(n=2,4,\dots)$ be the "orthogonal complement" of V_{n-2} in V_n, i.e., $V_n=W_n\oplus V_{n-2}$ (direct sum) and $W_n\perp V_{n-2}$, where orthogonality is defined by the natural inner product $(.,.)=\int(.)(.)\,\mathrm{d}\boldsymbol{n}/4\pi$. Then, W_n is a $2n+1$ dimensional subspace of V_n, and we obtain an orthogonal decomposition

$$V_n=W_n\oplus W_{n-2}\oplus\dots\oplus W_0. \tag{3.10}$$

If we take bases of W_m's as a basis of V_n, we obtain the desire expansion, and the coefficient tensors are determined independently of each other. This is just an extension of the "Schmidt orthogonalization" of the vectors 1, $n_i n_j, \ldots$ and $n_{i_1} \ldots n_{i_n}$. The decomposition (3.10) also has an interpretation in terms of the representation theory of the rotation group as follows.

Let $\boldsymbol{R}$ be a three dimensional rotation. Then, the space V_n is invariant to rotation $\boldsymbol{n} \to \boldsymbol{R}\boldsymbol{n}$, because $R_{i_1' i_1} \ldots R_{i_n' i_n} n_{i_1} \ldots n_{i_n}$ is again a vector of V_n. Therefore, a basis of V_n induces a "representation" $D^{(n+1)(n+2)/2}$ of the rotation group SO(3) of degree $(n+1)(n+2)/2$. As is well known, this representation is "completely reducible" and is reduced to the direct sum

$$D^{(n+1)(n+2)/2} = D_n \oplus D_{n-2} \oplus \cdots \oplus D_0, \tag{3.11}$$

where D_n is an "irreducible representation" of SO(3) of degree $2n+1$, and its representation space is just W_n in parallel with decomposition (3.10).

Let us briefly summarize the classical results. The "Laplace–Beltrami operator" on S^2 is $\Lambda = (1/\sin\theta)(\partial/\partial\theta)\sin\theta\,\partial/\partial\theta + (1/\sin^2\theta)\partial^2/\partial\phi^2$. (In terms of quantum mechanics, $-\hbar^2\Lambda$ is the "orbital angular momentum operator".) The subspace W_n is the eigenspace of Λ of eigenvalue $-n(n+1)$ and of multiplicity $2n+1$. Its vectors are called "spherical harmonics" of degree n (n is the "azimuthal quantum number" in quantum mechanics). Hence, two spherical harmonics with different n are mutually orthogonal. (One particular orthogonal basis of the same n is the "Laplace spherical harmonics" $Y_{nm}(\theta, \phi)$, and in quantum mechanics $m = -n, \ldots n$ is the "magnetic quantum number".) As is well known, these spherical harmonics constitute a complete set for expansion in the sense of $L^2(S^2)$.

4. FABRIC TENSORS OF THE THIRD KIND

Let us determine the subspace W_n discussed in the previous section. Let v be a vector of V_n. Since $v \in V_n$, it is expressed as a linear combination $c_{i_1\ldots i_n} n_{i_1} \ldots n_{i_n}$ of $n_{i_1} \ldots n_{i_n}$'s, where $c_{i_1\ldots i_n}$ is a symmetric tensor. The condition that $v \in W_n$ is $v \perp V_n$, i.e. $(v, n_{i_1} \ldots n_{i_{n-2}}) = 0$, where $(.,.) = \int (.)(.)\,d\boldsymbol{n}/4\pi$ is the natural inner product. This condition becomes

$$c_{j_1\ldots j_n} \overline{n_{j_1} \ldots n_{j_n} n_{i_1} \ldots n_{i_{n-2}}} = 0. \tag{4.1}$$

Contraction over $i_1 = i_2, \ldots$ and $i_{n-3} = i_{n-2}$ yields $c_{j_1\ldots j_n} \overline{n_{j_1} \ldots n_{j_n}} = 0$, which implies, in view of identity (3.4) and the symmetry of $c_{i_1\ldots i_n}$, that $c_{j_1 j_1 j_3 j_3 \ldots j_{n-1} j_{n-1}} = 0$. Combination of this and contraction of eqn (4.1) over $i_3 = i_4, \ldots$ and $i_{n-3} = i_{n-2}$ then yields $c_{j_1 j_1 j_3 j_3 \ldots j_{n-3} j_{n-3} i_1 i_2} = 0$, and so on. Thus, we can conclude that any contraction of $c_{i_1\ldots i_n}$ reduces to 0, or $c_{i_1\ldots i_n}$ is a "deviator tensor". Hence, W_n is included in a space spanned by $c_{i_1\ldots i_n} n_{i_1} \ldots n_{i_n}$'s with all deviator tensors $c_{i_1\ldots i_n}$. However, since $c_{i_1\ldots i_n}$ has only $2n+1$ independent components and the dimension of W_n is $2n+1$, these two spaces must coincide. Next, note that $c_{i_1\ldots i_n} n_{i_1} \ldots n_{i_n} = c_{i_1\ldots i_n} n_{\{i_1} \ldots n_{i_n\}}$, where {} designates the "deviator part" of a symmetric tensor. In other words, for a symmetric tensor $A_{i_1\ldots i_n}$,

$$A_{\{i_1\ldots i_n\}} = c_0^n A_{i_1\ldots i_n} + c_2^n \delta_{(i_1 i_2} A_{i_3\ldots i_n) j_1 j_1} + \cdots + c_n^n \delta_{(i_1 i_2} \delta_{i_3 i_4} \ldots \delta_{i_{n-1} i_n)} A_{j_1 j_1 j_3 j_3 \ldots j_{n-1} j_{n-1}}, \tag{4.2}$$

where $c_0^n = 1$ and $c_2^n, \ldots, c_n^n$ are determined in such a way that any contraction of $A_{\{i_1\ldots i_n\}}$ is zero. After some manipulation, we obtain

$$c_m^n = (-1)^{m/2} \binom{n}{m} \binom{n-1}{m/2} \Big/ \binom{2n-1}{m}. \tag{4.3}$$

Now, we have shown that W_n is a space spanned by $c_{i_1\ldots i_n} n_{i_1} \ldots n_{i_n}$'s with all deviator tensors $c_{i_1\ldots i_n}$, but it is the same as the space spanned by $c_{i_1\ldots i_n} n_{\{i_1} \ldots n_{i_n\}}$'s with all tensors $c_{i_1\ldots i_n}$, which implies that W_n is spanned by $n_{\{i_1} \ldots n_{i_n\}}$'s. Thus, the expansion takes the form

$$f(\boldsymbol{n}) = \frac{1}{4\pi}[D + D_{ij} n_{\{i} n_{j\}} + D_{ijkl} n_{\{i} n_j n_k n_{l\}} + \cdots]. \tag{4.4}$$

We call the coefficient tensor $D_{i_1 \dots i_n}$ the "fabric tensor of the third kind" of rank n. It is determined by the least square error method. Since each term is orthogonal to the rest, each coefficient is determined independently of the rest. By definition (4.4), $D_{i_1 \dots i_n}$ is determined as a deviator tensor. In view of eqn (3.4), it is concluded that

$$D_{i_1 \dots i_n} = \frac{2n+1}{2^n}\binom{2n}{n} N_{\{i_1 \dots i_n\}}. \tag{4.5}$$

Since $D_{i_1 \dots i_n}$ is a deviator tensor, expansion (4.4) is also written as

$$f(\boldsymbol{n}) = \frac{1}{4\pi}[D + D_{ij} n_i n_j + D_{ijkl} n_i n_j n_k n_l + \cdots]. \tag{4.6}$$

Example 4.1

$$D = 1, \tag{4.7}$$

$$D_{ij} = \frac{15}{2}\left[N_{ij} - \frac{1}{3}\delta_{ij}\right], \tag{4.8}$$

$$D_{ijkl} = \frac{315}{8}\left[N_{ijkl} - \frac{6}{7}\delta_{(ij}N_{kl)} + \frac{3}{35}\delta_{(ij}\delta_{kl)}\right], \tag{4.9}$$

$$D_{ijklmn} = \frac{3003}{16}\left[N_{ijklmn} - \frac{15}{11}\delta_{(ij}N_{klmn)} + \frac{5}{11}\delta_{(ij}\delta_{kl}N_{mn)} - \frac{5}{231}\delta_{(ij}\delta_{kl}\delta_{mn)}\right]. \tag{4.10}$$

Once $D_{ij}, \dots$ and $D_{i_1 \dots i_n}$ are known, we can compute $F_{i_1 \dots i_n}$ by "summing" them up:

$$F_{i_1 \dots i_n} = D_{i_1 \dots i_n} + \delta_{(i_1 i_2}D_{i_3 \dots i_n)} + \delta_{(i_1 i_2}\delta_{i_3 i_4}D_{i_5 \dots i_n)} + \cdots + \delta_{(i_1 i_2}\delta_{i_3 i_4} \cdots \delta_{i_{n-1} i_n)}. \tag{4.11}$$

Hence, the a^n_m's in eqn (3.6) are given by

$$a^n_m = \sum_{\substack{k=m \\ k:\text{even}}}^{n} \frac{2k+1}{2^k}\binom{2k}{k} c^k_{k-m} \Big/ \frac{2n+1}{2^n}\binom{2n}{n}. \tag{4.12}$$

Conversely, if $F_{i_1 \dots i_n}$'s are given, $D_{i_1 \dots i_n}$ is obtained by taking the "difference"

$$D_{i_1 \dots i_n} = F_{i_1 \dots i_n} - \delta_{(i_1 i_2}F_{i_3 \dots i_n)}. \tag{4.13}$$

In the next section, we show that $n_{\{i_1} \dots n_{i_n\}}$ is indeed a spherical harmonic of degree n. Hence, eqn (4.4) or (4.6) is nothing but the spherical harmonics expansion. The first term in eqn (4.4) or (4.6) is always 1, and the "normalization" $\int f(\boldsymbol{n})\,d\boldsymbol{n} = 1$ is always satisfied, because all the subsequent terms are orthogonal to 1. This illustrates the significance of the expansion (4.4) or (4.6) with respect to mutually orthogonal subspaces. Moreover, with this formulation, we can also make use of analogies with physical problems such as the potential theory in electrodynamics as is seen in the next section. This provides us with a physical interpretation of the tensor $D_{i_1 \dots i_n}$, which makes it easy to understand its intuitive meaning.

So far, we have discussed only the case of symmetric distributions. If the data are "truly directional" and the distribution is not symmetric, then we must add terms of $n_{i_1} \dots n_{i_n}$ of odd powers. However, subspaces V_1, V_3, ... are orthogonal to V_0, V_2, ... Hence, expansions in odd power terms can be treated independently of expansions in even power terms and is in complete parallel with that of even power terms, e.g. $n_{\{i_1} \dots n_{i_n\}}$ is a spherical harmonics of degree n for odd n, too.

5. MULTIPLE MOMENT EXPANSION AND MULTIPOLE MOMENT TENSORS

Consider the following problem. Suppose $f(\boldsymbol{n})$ is a surface charge density on a unit sphere located at the origin. Then, what is the electrostatic potential ϕ at a given point $\boldsymbol{r}$ far away from the sphere? If a unit point charge is placed at r', the potential at r is, as is well known, $1/\rho = 1/\|r - r'\| + \text{const.}$ (in esu). Let the arbitrary constant be zero. Since $\|r'\| \ll \|r\|$, it is approximated by a Taylor series with respect to r' around the origin

$$\frac{1}{\rho} = \sum_n \frac{1}{n!} \partial_{i_1'} \ldots \partial_{i_n'} \left(\frac{1}{\rho}\right)\bigg|_{r'=0} r'_{i_1} \ldots r'_{i_n}, \tag{5.1}$$

where ∂_i denotes $\partial/\partial r_i$. Note $\partial_{i_1'} \ldots \partial_{i_n'}(1/\rho)|_{r'=0} = (-1)^n \partial_{i_1} \ldots \partial_{i_n}(1/r)$. ($r = \|r\|$.) Now, the tensor $\partial_{i_1} \ldots \partial_{i_n}(1/r)$ is a homogeneous form of degree $-n-1$ in x, y and z and is a deviator tensor, because $1/r$ is a harmonic function, i.e. $\Delta(1/r) = 0$, where $\Delta = \partial_i \partial_i$ is the Laplacian operator. Comparing the coefficients and noting the uniqueness of the deviator part, we can conclude

$$\partial_{i_1} \ldots \partial_{i_n} \left(\frac{1}{r}\right) = \frac{(-1)^n (2n)!}{2^n n!} \frac{n_{\{i_1} \ldots n_{i_n\}}}{r^{n+1}}. \tag{5.2}$$

Since this is also a harmonic function, $n_{\{i_1} \ldots n_{i_n\}}/r^{n+1}$ is harmonic, and hence, as is well known, $r^n n_{\{i_1} \ldots n_{i_n\}}$ is also harmonic, which confirms that $n_{\{i_1} \ldots n_{i_n\}}$ is a spherical harmonic of degree n. Since both sides of eqn (5.2) is a deviator tensor, we can replace $r'_{i_1} \ldots r'_{i_n}$ in eqn (5.1) by its deviator part $r'_{\{i_1} \ldots r'_{i_n\}}$. Thus, we obtain a solution of the original potential problem in the form

$$\phi(r) = \int \frac{f(n)}{\|r - n\|} \mathrm{d}n = \sum_n \frac{Q_{i_1 \ldots i_n}}{n!} \frac{n_{i_1} \ldots n_{i_n}}{r^{n+1}}, \tag{5.3}$$

where

$$Q_{i_1 \ldots i_n} = \frac{(2n)!}{2^n n!} \langle n_{\{i_1} \ldots n_{i_n\}} \rangle \tag{5.4}$$

is what is usually referred to as the "multipole moment tensor". In particular, Q_{ij} is the "quadrupole moment tensor". Equation (5.3) is known as the "multipole moment expansion". Comparing eqn (5.4) and eqn (4.5), we can see

$$D_{i_1 \ldots i_n} = \frac{2n+1}{n!} Q_{i_1 \ldots i_n}, \tag{5.5}$$

if the observed data are interpreted as electric charges. Thus, eqn (4.6) is also interpreted as a multipole moment expansion, D_{ij} describing the quadrupole moment in particular. This also indicates the significance of using $D_{i_1 \ldots i_n}$ instead of $F_{i_1 \ldots i_n}$.

Some statisticians interpret the data as unit mass points on a unit sphere and calculate the "moment of inertia" to characterize the distribution[13]. It is expressed as a tensor $J_{ij} = N(\delta_{ij} - N_{ij})$ in our notation. This mechanical analogy also helps our intuitive understanding of the data distribution.

6. EXPANSION IN THE LAPLACE SPHERICAL HARMONICS

As was shown, $2n+1$ independent $n_{\{i_1} \ldots n_{i_n\}}$'s are spherical harmonics of degree n, but they are not mutually orthogonal. Of course, orthogonalization is possible, and one such orthogonal basis is the "Laplace spherical harmonics" $Y_{nm}(\theta, \phi)$, $m = -n, \ldots n$, defined by

$$Y_{nm}(\theta, \phi) = \sqrt{\frac{(2n+1)(n-m)!}{(n+m)!}} P_n^m(\cos\theta) e^{im\phi}, \tag{6.1}$$

for $m \geq 0$, and

$$Y_{n,-m}(\theta, \phi) = (-1)^m Y^*_{nm}(\theta, \phi), \tag{6.2}$$

for $m < 0$. Here, $P_n^m(x)$ is the "associated Legendre function", and $*$ denotes the complex conjugate. They are orthonormal, or "unitary" to be specific, in the sense of

$$\frac{1}{4\pi}\int Y_{nm}(\boldsymbol{n})Y^*_{n'm'}(\boldsymbol{n})\,d\boldsymbol{n} = \delta_{nn'}\delta_{mm'}, \tag{6.3}$$

and, as is well known, they form a complete orthonormal set on a unit sphere S^2 in L^2. Hence, we can use them for the expansion. However, we must fix a specific coordinate system, in reference to which the Laplace spherical harmonics are to be defined, and the expression is not invariant to coordinate rotations. Of course, transformation of spherical coordinates is possible, using the so called "addition theorem", but it does not have so simple a form as the tensor transformation. Still, if there is a preferred coordinate system, it is sometimes useful to express the expansion in terms of them. (For details, see [21], for example.) The expansion takes the form

$$f(\boldsymbol{n}) = \frac{1}{4\pi}\sum_{n=0}^{\infty}\sum_{m=-n}^{n} A_{nm}Y_{nm}(\boldsymbol{n}), \tag{6.4}$$

$$A_{nm} = \int f(\boldsymbol{n})Y^*_{nm}(\boldsymbol{n})\,d\boldsymbol{n}. \tag{6.5}$$

The expression of Y_{nm} as a homogeneous polynomial of degree n in x, y and z is obtained by expansion of the following "generating function" of Y_{nm}:

$$\frac{\sqrt{2n+1}}{n!t^n}\left(\frac{x-iy}{2}+zt-\frac{x+iy}{2}t^2\right)^n = \sum_{m=-n}^{n}\frac{Y_{nm}(\theta,\phi)t^m}{\sqrt{(n+m)!(n-m)!}}. \tag{6.6}$$

Example 6.1

Let $\boldsymbol{n} = (x, y, z)$. Then,

$$Y_{00} = 1, \tag{6.7}$$

$$\begin{aligned}
&Y_{22} = \frac{\sqrt{30}}{4}(x^2+2ixy-y^2), \quad Y_{21} = -\frac{\sqrt{30}}{2}(xz+iyz),\\
&Y_{20} = -\frac{\sqrt{5}}{2}(x^2+y^2-2z^2), \quad Y_{2,-1} = -Y^*_{21}, \quad Y_{2,-2} = Y^*_{22},
\end{aligned} \tag{6.8}$$

$$\begin{aligned}
&Y_{44} = \frac{3\sqrt{70}}{16}(x^4+4ix^3y-6x^2y^2-4ixy^3+y^4),\\
&Y_{43} = -\frac{3\sqrt{35}}{4}(x^3z+3ix^2yz-3xy^2z-iy^3z),\\
&Y_{42} = -\frac{3\sqrt{10}}{8}(x^4+2ix^3y-6x^2z^2+2ixy^3-12ixyz^2-y^4+6y^2z^2),\\
&Y_{41} = \frac{3\sqrt{5}}{4}(3x^3z+3ix^2yz+3xy^2z-4xz^3+3iy^3z-4iyz^3),\\
&Y_{40} = \frac{3}{8}(3x^4+6x^2y^2-24x^2z^2+3y^4-24y^2z^2+8z^4).
\end{aligned} \tag{6.9}$$

The expansion coefficients are given by $A_{nm} = \langle Y^*_{nm}(\boldsymbol{n})\rangle$ from eqn (6.5). Hence, they are expressed as linear combinations of $N_{i_1\ldots i_n}$'s.

Example 6.2

$$A_{00} = 1, \tag{6.10}$$

$$\begin{aligned}
&A_{22} = \frac{\sqrt{30}}{4}(N_{11}-2iN_{12}-N_{22}), \quad A_{21} = -\frac{\sqrt{30}}{2}(N_{13}-iN_{23}),\\
&A_{20} = -\frac{\sqrt{5}}{2}(N_{11}+N_{22}-2N_{33}), \quad A_{2,-1} = -A^*_{21}, \quad A_{2,-2} = A^*_{22},
\end{aligned} \tag{6.11}$$

$$A_{44} = \frac{3\sqrt{70}}{16}(N_{1111} - 4iN_{1112} - 6N_{1122} + 4iN_{1222} + N_{2222}),$$

$$A_{43} = -\frac{3\sqrt{35}}{4}(N_{1113} - 3iN_{1123} - 3N_{1223} + iN_{2223}),$$

$$A_{42} = -\frac{3\sqrt{10}}{8}(N_{1111} - 2iN_{1112} - 6N_{1133} - 2iN_{1222} + 12iN_{1233} - N_{2222} + 6N_{2333}),$$

$$A_{41} = \frac{3\sqrt{5}}{4}(3N_{1113} - 3iN_{1123} + 3N_{1223} - 4N_{1333} - 3iN_{2223} + 4iN_{2333}),$$

$$A_{40} = \frac{3}{8}(3N_{1111} + 6N_{1122} - 24N_{1133} + 3N_{2222} - 24N_{2233} + 8N_{3333}). \tag{6.12}$$

However, it is easier to express Y_{nm}'s and A_{nm}'s in terms of $n_{\{i_1} \ldots n_{i_n\}}$'s and $D_{i_1 \ldots i_n}$'s, because the following identity is available:

$$(\partial_x + i\partial_y)^m \partial_z^{n-m}\left(\frac{1}{r}\right) = \frac{(-1)^n}{r^{n+1}}\sqrt{\frac{(n+m)!(n-m)!}{2n+1}}\,Y_{nm}(\theta, \phi), \tag{6.13}$$

($m \geq 0$). Hence, in view of eqn (5.2), we obtain for $m \geq 0$

$$Y_{nm}(\theta, \phi) = \frac{(2n)!}{2^n n!}\sqrt{\frac{2n+1}{(n+m)!(n-m)!}}\sum_{k=0}^{m}(i)^{m-k}\binom{m}{k}\overbrace{n_{\{1}\ldots}^{k}\overbrace{n_2\ldots}^{m-k}\overbrace{n_3\ldots n_{3\}}}^{n-m}, \tag{6.14}$$

$$A_{nm} = \frac{n!}{\sqrt{(2n+1)(n+m)!(n-m)!}}\sum_{k=0}^{m}(-i)^{m-k}\binom{m}{k}D_{\overbrace{1\ldots1}^{k}\overbrace{2\ldots2}^{m-k}\overbrace{3\ldots3}^{n-m}} \tag{6.15}$$

Example 6.3

$$A_{22} = \frac{\sqrt{30}}{30}(D_{11} - 2iD_{12} - D_{22}),\quad A_{21} = \frac{\sqrt{30}}{15}(D_{13} - iD_{33}),\quad A_{20} = \frac{\sqrt{5}}{5}D_{33}, \tag{6.16}$$

$$A_{44} = \frac{\sqrt{70}}{210}(D_{1111} - 4iD_{1112} - 6D_{1122} + 4iD_{1222} + D_{2222}),$$

$$A_{43} = \frac{2\sqrt{35}}{105}(D_{1113} - 3iD_{1123} - 3D_{1223} + iD_{2223}),$$

$$A_{42} = \frac{\sqrt{10}}{15}(D_{1133} - 2iD_{1233} - D_{2233}),$$

$$A_{41} = \frac{2\sqrt{5}}{15}(D_{1333} - iD_{2333}),\quad A_{40} = \frac{1}{3}D_{3333}. \tag{6.17}$$

This also illustrates the importance of the tensor $D_{i_1 \ldots i_n}$.

7. TWO DIMENSIONAL DATA DISTRIBUTIONS

Now, the previous results are adapted to two dimensional data distributions. Here again $V_0 \subset V_2 \subset V_4 \subset \ldots$, where V_n is the vector space of functions on S^1 spanned by $n_{i_1} \ldots n_{i_n}$'s and its dimension is $n+1$ (consider the number of 1's among $i_1, \ldots, i_n$). For the same reason as before, it is sufficient to seek an approximation in the form

$$f(\boldsymbol{n}) \sim \frac{1}{2\pi}F_{i_1 \ldots i_n}n_{i_1} \ldots n_{i_n}. \tag{7.1}$$

The coefficients are again determined by eqn (3.3), but identity (3.4) is replaced by

$$\overline{n_{i_1}n_{i_2} \ldots n_{i_{2n}}} = \frac{1}{2^{2n}}\binom{2n}{n}\delta_{(i_1 i_2}\delta_{i_3 i_4} \ldots \delta_{i_{2n-1} i_{2n})}. \tag{7.2}$$

Then, the "fabric tensor of the second kind" also takes the form

$$F_{i_1\dots i_n} = 2^n[N_{i_1\dots i_n} + a^n_{n-2}\delta_{(i_1i_2}N_{i_3\dots i_n)} + \cdots + a^n_0\delta_{(i_1i_2}\delta_{i_3i_4}\dots\delta_{i_{n-1}i_n)}]. \tag{7.3}$$

Example 7.1

$$F = 1, \tag{7.4}$$

$$F_{ij} = 4\left[N_{ij} - \frac{1}{4}\delta_{ij}\right], \tag{7.5}$$

$$F_{ijkl} = 16\left[N_{ijkl} - \frac{3}{4}\delta_{(ij}N_{kl)} + \frac{1}{16}\delta_{(ij}\delta_{kl)}\right], \tag{7.6}$$

$$F_{ijklmn} = 64\left[N_{ijklmn} - \frac{5}{4}\delta_{(ij}N_{klmn)} + \frac{3}{8}\delta_{(ij}\delta_{kl}N_{mn)} - \frac{1}{64}\delta_{(ij}\delta_{kl}\delta_{mn)}\right]. \tag{7.7}$$

Again, the same discussion applies, and we can obtain the decomposition (3.10), where orthogonality is defined by the natural inner product $(.,.) = \int (.)(.)\,d\boldsymbol{n}/2\pi$. Then, W_n is obtained as a two dimensional subspace of V_n. The interpretation in terms of the representation theory of the rotation group remains the same except that a representation E^{n+1} of the two dimensional rotation group SO(2) of degree $n+1$ in V_n is decomposed into the direct sum

$$E^{n+1} = E_n \oplus E_{n-2} \oplus \cdots \oplus E_0, \tag{7.8}$$

where E_n $(n>0)$ is an irreducible representation (in the real domain) of SO(2) of degree 2 and E_0 is the unit representation of degree 1. (In the complex domain, E_n $(n>0)$ is further decomposed into two representations of degree 1, $E_n = E_{+n} \oplus E_{-n}$.) The subspace W_n coincides with the representation space of E_n and is also the eigenspace of the two dimensional "Laplace–Beltrami operator" $d^2/d\theta^2$ of eigenvalue $-n^2$ and of multiplicity 2. Its vectors are "circular harmonics" or "trigonometric functions" of degree n. Hence, circular harmonics of different n are mutually orthogonal, and they form a complete set for the expansion in $L^2(S^1)$. One particular orthogonal basis of the same n is, of course, the "Fourier" circular harmonics $e^{in\theta}$ and $e^{-in\theta}$. As in the three dimensional case, the deviator part $n_{\{i_1}\dots n_{i_n\}}$ spans the subspace W_n, and $f(\boldsymbol{n})$ is expanded in the form

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[D + D_{ij}n_{\{i}n_{j\}} + D_{ijkl}n_{\{i}n_jn_kn_{l\}} + \cdots]. \tag{7.9}$$

The deviator part $\{\}$ is again defined by eqn (4.2), but, instead of eqn (4.3), c^n_m's are given by

$$c^n_m = \frac{(-1)^{m/2}}{2^m}\frac{n}{n-m/2}\binom{n-m/2}{m/2}. \tag{7.10}$$

The "fabric tensor of the third kind" is given by

$$D_{i_1\dots i_n} = 2^nN_{\{i_1\dots i_n\}}. \tag{7.11}$$

Example 7.2

$$D = 1, \tag{7.12}$$

$$D_{ij} = 4\left[N_{ij} - \frac{1}{2}\delta_{ij}\right], \tag{7.13}$$

$$D_{ijkl} = 16\left[N_{ijkl} - \delta_{(ij}N_{kl)} + \frac{1}{8}\delta_{(ij}\delta_{kl)}\right], \tag{7.14}$$

$$D_{ijklmn} = 64\left[N_{ijklmn} - \frac{3}{2}\delta_{(ij}N_{klmn)} + \frac{9}{16}\delta_{(ij}\delta_{kl}N_{mn)} - \frac{1}{32}\delta_{(ij}\delta_{kl}\delta_{mn)}\right]. \tag{7.15}$$

Since $D_{i_1\ldots i_n}$ is a deviator tensor, expansion (7.9) is also written as

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[D + D_{ij}n_in_j + D_{ijkl}n_in_jn_kn_l + \cdots], \tag{7.16}$$

and $D = 1$ so that normalization $\int f(\boldsymbol{n})\,\mathrm{d}\boldsymbol{n} = 1$ is always satisfied. However, as we noted earlier, $D_{i_1\ldots i_n}$ has only two independent components. Let $D_{1\ldots 1} = a_n$ and $D_{1\ldots 12} = b_n$, for example. Then,

$$D_{1\ldots \overbrace{12\ldots 2}^{k}} = \begin{cases} (-1)^{k/2}a_n & k\text{: even} \\ (-1)^{(k-1)/2}b_n & k\text{: odd} \end{cases} \tag{7.17}$$

Expansion (7.9) or (7.16) is nothing but the Fourier series, and a_n and b_n are its Fourier coefficients. Namely, expansion (7.9) or (7.16) is rewritten as a Fourier series

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[1 + a_2\cos 2\theta + b_2\sin 2\theta + a_4\cos 4\theta + b_4\sin 4\theta + \cdots]. \tag{7.18}$$

Since the general form of $D_{i_1\ldots i_n}$ is known, the general form of $F_{i_1\ldots i_n}$ is obtained by the summation of eqn (4.11). Equation (4.12) is now replaced by

$$a_m^n = \frac{1}{2^n}\sum_{\substack{k=m \\ k:\text{even}}}^{n} 2^k c_{k-m}^k. \tag{7.19}$$

Conversely, if $F_{i_1\ldots i_n}$'s are given, $D_{i_1\ldots i_n}$ is obtained by the difference of eqn (4.13).

The electrostatic potential analogy in Section 5 becomes as follows. Here, a two dimensional point charge in the $x-y$ plane is actually an infinitely long charged line with unit line density of charge extending parallel to the z-axis. Let $f(\boldsymbol{n})$ be a line charge density on a unit circle located at the origin in the $x-y$ plane. (Actually, of course, it is a surface charge density on an infinitely long cylinder extending vertically.) If a (two dimensional) unit point charge is placed at $\boldsymbol{r}'$, the potential at $\boldsymbol{r}$ is $2\log(1/\rho) + \text{const.}$ (in esu), where $\rho = \|\boldsymbol{r} - \boldsymbol{r}'\|$. We choose the arbitrary constant to be 1 so that the potential equals 1 at $\rho = 1$. If $\|\boldsymbol{r}'\| \ll \|\boldsymbol{r}\|$, the Taylor expansion is available in the form

$$\log\frac{1}{\rho} = \sum_n \frac{1}{n!}\partial_{i_1'}\cdots\partial_{i_n'}\log\left(\frac{1}{\rho}\right)\bigg|_{r'=0} r'_{i_1}\cdots r'_{i_n}, \tag{7.20}$$

and $\partial_{i_1'}\cdots\partial_{i_n'}\log(1/\rho)|_{r'=0} = (-1)^n\partial_{i_1}\cdots\partial_{i_n}\log(1/r)$. We can easily show that

$$\partial_{i_1}\cdots\partial_{i_n}\log\frac{1}{r} = (-1)^n 2^{n-1}(n-1)!\,\frac{n_{\{i_1}\cdots n_{i_n\}}}{r^n}. \tag{7.21}$$

Since this is a harmonic function, $n_{\{i_1}\cdots n_{i_n\}}/r^n$ is harmonic, and hence $r^n n_{\{i_1}\cdots n_{i_n\}}$ is also harmonic, which means $n_{\{i_1}\cdots n_{i_n\}}$ is a circular harmonic or a trigonometric function of degree n. As in the three dimensional case, the solution of the original potential problem is

$$\phi(\boldsymbol{r}) = \int f(\boldsymbol{n})\left(1 + 2\log\frac{1}{\|\boldsymbol{r}-\boldsymbol{n}\|}\right)\mathrm{d}\boldsymbol{n} = \sum_n \frac{Q_{i_1\ldots i_n}}{n!}\frac{n_{i_1}\cdots n_{i_n}}{r^n}, \tag{7.22}$$

where the "multipole moment tensor" is given by

$$Q_{i_1\ldots i_n} = 2^n(n-1)!\,n_{\{i_1}\cdots n_{i_n\}}, \tag{7.23}$$

for $n > 0$ and $Q = 1$ for $n = 0$. Hence, we can see that

$$D_{i_1\ldots i_n} = \frac{1}{(n-1)!}Q_{i_1\ldots i_n}. \tag{7.24}$$

As was remarked earlier, a particular orthogonal basis of W_n is the "Fourier" circular harmonics $e^{in\theta} = \cos n\theta + i \sin n\theta$ and $e^{-in\theta} = \cos n\theta - i \sin n\theta$. The complex Fourier series expansion takes the form

$$f(\boldsymbol{n}) = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} A_n \, e^{in\theta}, \tag{7.25}$$

$$A_n = \int f(\boldsymbol{n}) \, e^{-n\theta} \, d\boldsymbol{n} = \langle e^{-in\theta} \rangle. \tag{7.26}$$

Since $e^{in\theta} = (x + iy)^n$ and $e^{-in\theta} = (x - iy)^n$, we can see that $e^{2i\theta} = x^2 + 2ixy - y^2$, $e^{-2i\theta} = x^2 - 2ixy - y^2$, etc. corresponding to Example 6.1. Corresponding to Example 6.2 are $A_0 = 1$, $A_2 = N_{11} - 2iN_{12} - N_{22}$, $A_{-2} = A_2^*$, etc. The two dimensional version of eqn (6.13) is

$$(\partial_x + i\partial_y)^n \log \frac{1}{r} = (-1)^n 2^{n-1} (n-1)! \frac{e^{in\theta}}{r^n}, \tag{7.27}$$

for $n > 0$, and hence eqns (6.14) and (6.15) become

$$e^{in\theta} = \sum_{k=0}^{n} (i)^{n-k} \binom{n}{k} \overbrace{n_{\{1} \ldots}^{k} n_2 \ldots n_{2\}}, \tag{7.28}$$

$$A_n = \frac{1}{2^n n!} \sum_{k=0}^{n} (-i)^{n-k} \binom{n}{k} D_{\overbrace{1 \ldots}^{k} 2 \ldots 2}, \tag{7.29}$$

and $A_{-n} = A_n^*$ for $n > 0$. Corresponding to Example 6.4 are $A_2 = (D_{11} - 2iD_{12} - D_{22})/8$, etc.

8. STATISTICAL TEST FOR THE FITNESS OF THE DISTRIBUTION

Since $n_{\{i_1} \ldots n_{i_n\}}$'s form a complete basis in L^2 on S^2 or S^1, the expansion of an empirical density $f(\boldsymbol{n})$ converges in the limit to the original $f(\boldsymbol{n})$, while our aim is to characterize $f(\boldsymbol{n})$ by a smooth function with certain physical meaning. Therefore, only a small number of terms need be retained, but how many of them are sufficient? In order to answer this question, we must resort to a statistical test.

The simplest problem is the "test of uniformity". Suppose the computed D_{ij} is very small and the distribution is almost "uniform" or "isotropic", i.e. $f(\boldsymbol{n}) \sim 1/4\pi$ in the three dimensional case or $f(\boldsymbol{n}) \sim 1/2\pi$ in the two dimensional case. Then, how small should D_{ij} be in order to conclude that the true population is uniform and that the computed non-zero D_{ij} is a statistical fluctuation due to the finite size of the data? This problem is solved by calculating the "likelihood ratio", i.e. the probability that the observed data are generated by the uniform distribution over the probability that the observed data are generated by the distribution calculated up to the term of D_{ij}. If this ratio is too small, we cannot conclude that the true population is uniform. Then, the second term must be retained. The same process also applies to higher terms. For example, in order to test whether the term of D_{ijkl} can be neglected or not, we compute the likelihood ratio with respect to the distribution up to the term of D_{ij} vs the distribution up to the term of D_{ijkl}, and so on.

Let λ be the likelihood ratio. It is known that $-2 \log \lambda$ behaves according to the χ^2-distribution, its degree of freedom being the number of independent parameters whose nullity is to be tested, if the number N of independently observed data is sufficiently large. It is also known that $-2 \log \lambda$ is expressed as a quadratic form of the parameters to be tested, the coefficient being N times the "Fisher information matrix", if N is sufficiently large. (Strictly speaking, these results apply when the distribution is estimated by the "maximum likelihood estimation", not the "least square error approximation", but the difference is not so significant if N is sufficiently large. For details, see [22], for example.)

First, consider the test of uniformity. Let $F(\boldsymbol{n})$ be the distribution calculated up to the second term from independently observed N data:

$$F(\boldsymbol{n}) = \frac{1}{4\pi}[1 + D_{ij} n_i n_j] \quad \text{or} \quad \frac{1}{2\pi}[1 + D_{ij} n_i n_j], \tag{8.1}$$

for the three and two dimensional cases respectively. The Fisher information matrix in this case is a tensor defined by

$$I_{ijkl} = \int \frac{1}{F} \frac{\partial F}{\partial D_{ij}} \frac{\partial F}{\partial D_{kl}} \, d\boldsymbol{n}|_{D_{mn}=0}. \tag{8.2}$$

Substitution of eqn (8.1) yields

$$I_{ijkl} = \frac{1}{5} \delta_{(ij}\delta_{kl)} \quad \text{or} \quad \frac{3}{8} \delta_{(ij}\delta_{kl)}, \tag{8.3}$$

respectively. The statistics to be tested is $NI_{ijkl}D_{ij}D_{kl}$, or

$$\frac{2N}{15} D_{ij}D_{ij} \quad \text{or} \quad \frac{N}{4} D_{ij}D_{ij}, \tag{8.4}$$

respectively. Let $\chi_c^2(p, \alpha)$ be the value of χ^2 whose upper probability is α, i.e. $\text{Prob}\{\chi^2 > \chi_c^2(p, \alpha)\} = \alpha$, χ^2 obeying the χ^2-distribution of degree of freedom p. If the value of (8.4) is larger than $\chi_c^2(5, \alpha)$ or $\chi_c^2(2, \alpha)$ respectively, the observation is "significant", i.e. the distribution cannot be regarded uniform, under "significance level" α. If we express the latter of (8.4) in terms of the Fourier coefficients a_2 and b_2 (see eqns (7.16) and (7.17)), it becomes $N(a_2^2 + b_2^2)/2$.

A test for D_{ijkl} is obtained similarly. Let

$$F(\boldsymbol{n}) = \frac{1}{4\pi}[1 + D_{ij}n_in_j + D_{ijkl}n_in_jn_kn_l] \quad \text{or} \quad \frac{1}{2\pi}[1 + \cdots] \tag{8.5}$$

be the distribution calculated up to the term of D_{ijkl}. The Fisher information in this case is

$$I_{ijklmnpq} = \int \frac{1}{F} \frac{\partial F}{\partial D_{ijkl}} \frac{\partial F}{\partial D_{mnpq}} \, d\boldsymbol{n}|_{D_{rstu}=0}. \tag{8.6}$$

This integration does not yield a simple form. If we expand it in D_{ij} and retain only 0th and first terms of D_{ij}, assuming D_{ij} is small compared to 1, we obtain

$$NI_{ijklmnpq}D_{ijkl}D_{mnpq} = \begin{cases} \dfrac{8N}{315}\left[D_{ijkl}D_{ijkl} - \dfrac{8}{11} D_{ijkl}D_{ijkm}D_{lm}\right] \\[2ex] \dfrac{N}{16} D_{ijkl}D_{ijkl} \end{cases}, \tag{8.7}$$

for the three and the two dimensional cases respectively. (Note that $D_{ijkl}D_{ijkm}D_{lm} = 0$ in the two dimensional case. See eqn (7.17). The statistic becomes again $N(a_4^2 + b_4^2)/2$ in terms of the Fourier coefficients.) This statistic is tested against $\chi_c^2(9, \alpha)$ or $\chi_c^2(2, \alpha)$ respectively as before.

We can also estimate the deviation, due to the finite size of data, of computed D_{ij} and D_{ijkl} from D_{ij}^0 and D_{ijkl}^0 respectively of the true population distribution by noting that $(D_{ij} - D_{ij}^0)/\sqrt{N}$'s and $(D_{ijkl} - D_{ijkl}^0)/\sqrt{N}$'s obey the multivariate normal distribution with mean 0 and with variance the inverse of the respective Fisher information matrix when N is sufficiently large.

9. AN EXAMPLE OF CHARACTERIZING AND TESTING DISTRIBUTIONS

As an example, let us consider the interparticle contact distribution of granular materials. Figures 1 and 2 show circular histograms ("rose diagrams") of the contact directions in an assembly of oval rods (a two-dimensional granular material) observed by Konishi *et al.* [16]. The x- and y-axes are taken to coincide with the principal stress axes of the external loading. Figure 1 describes the distribution before the loading and Fig. 2 after the loading. Let us try to quantify

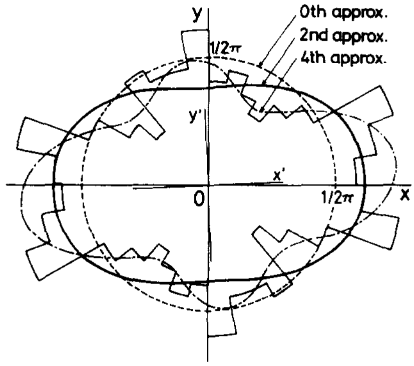

Fig. 1. The contact distribution of a two dimensional granular material (before loading).

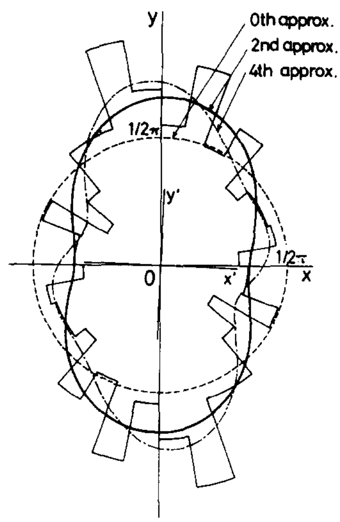

Fig. 2. The contact distribution of a two dimensional granular material (after loading).

this change of the packing configuration. First, consider the case of Fig. 1. The fabric tensors of the first kind become as follows:

$$\begin{aligned} &N_{11}=0.5605, && N_{12}=0.005328, && N_{22}=0.4395,\\ &N_{1111}=0.4483, && N_{1112}=0.01029, && N_{1122}=0.1122,\\ &N_{1222}=-0.004965, && N_{2222}=0.3273, \text{etc.} && \end{aligned} \tag{9.1}$$

The fabric tensors of the second kind are

$$\begin{aligned} &F_{11}=1.242, && F_{12}=0.02131, && F_{22}=0.7579,\\ &F_{1111}=1.447, && F_{1112}=0.1327, && F_{1122}=0.1282,\\ &F_{1222}=-0.1114, && F_{2222}=0.9631, \text{etc.}, && \end{aligned} \tag{9.2}$$

which implies that the distribution density is approximated as follows:

$$\begin{aligned} &f(\boldsymbol{n})\sim\frac{1}{2\pi} && \text{(0th order)},\\ &f(\boldsymbol{n})\sim\frac{1}{2\pi}[1.242x^2+0.04262xy+0.7579y^2] && \text{(2nd order)},\\ &f(\boldsymbol{n})\sim\frac{1}{2\pi}[1.447x^4+0.5308x^3y+0.7692x^2y^2-0.4456xy^3+0.9631y^4] && \text{(4th order)}. \end{aligned} \tag{9.3}$$

The corresponding approximated distributions are drawn over the rose diagram in the Fig. 1. The fabric tensors of the third kind are

$$D_{11} = 0.2421, \quad D_{12} = 0.02131, \quad D_{22} = -0.2421,$$
$$D_{1111} = 0.2052, \quad D_{1112} = 0.1221, \quad D_{1122} = -0.2052,$$
$$D_{1222} = -0.1221, \quad D_{2222} = 0.2052, \text{ etc.} \tag{9.4}$$

This means that the distribution density is approximated by

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[1 + 0.2421(x^2 - y^2) + 0.04262xy + 0.2052(x^4 - 6x^2y^2 + y^4) + 0.4884(x^3y - xy^3) + \cdots], \tag{9.5}$$

which can be extended up to any desired order. In fact, this expression corresponds to the following Fourier series:

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[1 + 0.2421 \cos 2\theta + 0.02131 \sin 2\theta + 0.2052 \cos 4\theta + 0.1221 \sin 4\theta + \cdots]. \tag{9.6}$$

The eigenvalues of N_{ij} are 0.5607 and 0.4393, and the angles made by their eigenvectors and the x-axis are 2.51° and 92.52° respectively. Hence, if they are taken respectively as the new x'- and y'-axes, the transformed fabric tensors are

$$N_{i'j'} = \begin{bmatrix} 0.5607 & 0 \\ 0 & 0.4393 \end{bmatrix}, \tag{9.7}$$

$$F_{i'j'} = \begin{bmatrix} 1.243 & 0 \\ 0 & 0.7572 \end{bmatrix}, \tag{9.8}$$

$$D_{i'j'} = \begin{bmatrix} 0.2428 & 0 \\ 0 & -0.2428 \end{bmatrix}, \tag{9.9}$$

and the transformed approximation is

$$f(\boldsymbol{n}) = \frac{1}{2\pi}[1 + 0.2428(x'^2 - y'^2) + 0.2233(x'^4 - 6x'^2y'^2 + y'^4) + 0.3374(x'^3y' - x'y'^3) + \cdots]. \tag{9.10}$$

The same analysis can be done for Fig. 2, and approximations up to the fourth order are also plotted in it.

Let us test the uniformity of the distribution. The statistic $ND_{ij}D_{ij}/4$ $(=N(a_2^2 + b_2^2)/2)$ becomes 17.04 for Fig. 1 and 26.53 for Fig. 2. (The number of the data, N, is 577 for the former and 527 for the latter.) Since $\chi_c^2(2, 0.005) = 10.60$, both of them are "significant", i.e. they cannot be regarded as data from the uniform distribution, with significance level 0.005. Next, consider the term of D_{ijkl}. Since the statistic $ND_{ijkl}D_{ijkl}/16$ $(= N(a_4^2 + b_4^2)/2)$ becomes 16.44 for Fig. 1 and 6.201 for Fig. 2, the former is "significant" while the latter is not, i.e. the term of D_{ijkl} cannot be neglected for Fig. 1 but it can be neglected for Fig. 2, with significance level 0.005.

It is conjectured that the principal axes of the fabric tensors of rank 2 (of any kind) coincide with the principal stress axes. If they are assumed to be related to the stress tensor, then we can think of various possibilities [5, 6, 9–11]. Since $N_{kk} = 1$, $F_{kk} = 3$ or 2 (for the three and the two dimensional cases, respectively) and $D_{kk} = 0$, some simple forms are

$$N_{ij} = \sigma_{ij}/\sigma_{kk}, \tag{9.11}$$

$$F_{ij} = 3\sigma_{ij}/\sigma_{kk} \text{ or } 2\sigma_{ij}/\sigma_{kk}, \text{ respectively}, \tag{9.12}$$

$$D_{ij} = \text{const. } \sigma_{\{ij\}}. \tag{9.13}$$

Kanatani [6, 12] assumed eqn (9.12), because in this case the distribution density approximated up to the second order does not take negative values as long as the stress is in a compressive state, i.e. σ_{ij} is positive definite. In this connection, Satake[11] proposed a form of the distribution density which yields the prescribed fabric tensor of rank 2 and is always positive. However, his form is very much complicated, involving the eigenvalues of the fabric tensor and the polar coordinates of its principal axes, so that physical interpretations or analogies and statistical tests are difficult to apply.

The validity of the assumptions of eqns (9.11)–(9.13) must be judged from further experimental observations, of course, but this illustrates how the analysis of this paper provides us with useful tools to cope with this kind of problems. In the above example, we considered the stress tensor as an external control factor. It is clear that if quantities of higher ranks are involved, fabric tensors of higher ranks should be also taken into consideration. We can also see advantages of the use of fabric tensors over the use of spherical harmonics or Fourier coefficients. The fabric tensors are calculated systematically without any reference to special functions. Moreover, since they are tensors, they not only have a simple rule for transformations of the coordinate system but also can be directly employed in describing the physical laws governing the phenomenon, which should be expressed as tensor equations. At the same time, we can easily understand the intuitive meaning of these tensors in connection with the form of the distribution density, because the expansion corresponds to the multipole moment expansion and each $D_{i_1\ldots i_n}$ describes the amount of the corresponding multipole moment.

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