Information Geometry: Near Randomness and Near Independence

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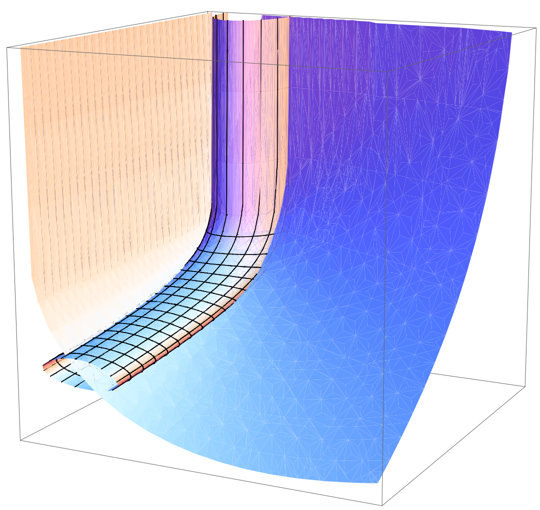

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Preface

The main motivation for this book lies in the breadth of applications in which a statistical model is used to represent small departures from, for example, a Poisson process. Our approach uses information geometry to provide a common context but we need only rather elementary material from differential geometry, information theory and mathematical statistics. Introductory sections serve together to help those interested from the applications side in making use of our methods and results. We have available *Mathematica* notebooks to perform many of the computations for those who wish to pursue their own calculations or developments.

Some 44 years ago, the second author first encountered, at about the same time, differential geometry via relativity from Weyl's book [209] during undergraduate studies and information theory from Tribus [200, 201] via spatial statistical processes while working on research projects at Wiggins Teape Research and Development Ltd—cf. the Foreword in [196] and [170, 47, 58]. Having started work there as a student laboratory assistant in 1959, this research environment engendered a recognition of the importance of international collaboration, and a lifelong research interest in randomness and near-Poisson statistical geometric processes, persisting at various rates through a career mainly involved with global differential geometry. From correspondence in the 1960s with Gabriel Kron [4, 124, 125] on his Diakoptics, and with Kazuo Kondo who influenced the post-war Japanese schools of differential geometry and supervised Shun-ichi Amari's doctorate [6], it was clear that both had a much wider remit than traditionally pursued elsewhere. Indeed, on moving to Lancaster University in 1969, receipt of the latest *RAAG Memoirs Volume 4 1968* [121] provided one of Amari's early articles on information geometry [7], which subsequently led to his greatly influential 1985 Lecture Note volume [8] and our 1987 *Geometrization of Statistical Theory Workshop* at Lancaster University [10, 59].

Reported in this monograph is a body of results, and computer-algebraic methods that seem to have quite general applicability to statistical models admitting representation through parametric families of probability density functions. Some illustrations are given from a variety of contexts for geometric characterization of statistical states near to the three important standard basic reference states: (Poisson) randomness, uniformity, independence. The individual applications are somewhat heuristic models from various fields and we incline more to terminology and notation from the applications rather than from formal statistics. However, a common thread is a geometrical representation for statistical perturbations of the basic standard states, and hence results gain qualitative stability. Moreover, the geometry is controlled by a metric structure that owes its heritage through maximum likelihood to information theory so the quantitative features—lengths of curves, geodesics, scalar curvatures etc.—have some respectable authority. We see in the applications simple models for galactic void distributions and galaxy clustering, amino acid clustering along protein chains, cryptographic protection, stochastic fibre networks, coupled geometric features in hydrology and quantum chaotic behaviour. An ambition since the publication by Richard Dawkins of *The Selfish Gene* [51] has been to provide a suitable differential geometric framework for dynamics of natural evolutionary processes, but it remains elusive. On the other hand, in application to the statistics of amino acid spacing sequences along protein chains, we describe in Chapter 7 a stable statistical qualitative property that may have evolutionary significance. Namely, to widely varying extents, all twenty amino acids exhibit greater clustering than expected from Poisson processes. Chapter 11 considers eigenvalue spacings of infinite random matrices and near-Poisson quantum chaotic processes.

The second author has benefited from collaboration (cf. [34]) with the group headed by Andrew Doig of the Manchester Interdisciplinary Biocentre, the University of Manchester, and has had long-standing collaborations with groups headed by Bill Sampson of the School of Materials, the University of Manchester (cf.eg. [73]) and Jacob Scharcanski of the Instituto de Informatica, Universidade Federal do Rio Grande do Sul, Porto Alegre, Brasil (cf.eg. [76]) on stochastic modelling. We are pleased therefore to have co-authored with these colleagues three chapters: titled respectively, Amino Acid Clustering, Stochastic Fibre Networks, Stochastic Porous Media and Hydrology.

The original draft of the present monograph was prepared as notes for short Workshops given by the second author at Centro de Investigaciones de Matematica (CIMAT), Guanajuato, Mexico in May 2004 and also in the Departamento de Xeometra e Topoloxa, Facultade de Matemáticas, Universidade de Santiago de Compostela, Spain in February 2005.

The authors have benefited at different times from discussions with many people but we mention in particular Shun-ichi Amari, Peter Jupp, Patrick Laycock, Hiroshi Matsuzoe, T. Subba Rao and anonymous referees. However, any overstatements in this monograph will indicate that good advice may have been missed or ignored, but actual errors are due to the authors alone.

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Contents

Here below are the opening pages for the chapters, and the References.
MSC(2000): 53B50, 60D05, 62B10, 62P35, 74E35, 92D20

1

Mathematical Statistics and Information Theory

There are many easily found good books on probability theory and mathematical statistics (eg [84, 85, 87, 117, 120, 122, 196]), stochastic processes (eg [31, 161]) and information theory (eg [175, 176]); here we just outline some topics to help make the sequel more self contained. For those who have access to the computer algebra package *Mathematica* [215], the approach to mathematical statistics and accompanying software in Rose and Smith [177] will be particularly helpful.

The word stochastic comes from the Greek *stochastikos*, meaning skillful in aiming and *stochazesthai* to aim at or guess at, and *stochos* means target or aim. In our context, stochastic colloquially means involving chance variations around some event—rather like the variation in positions of strikes aimed at a target. In its turn, the later word statistics comes through eighteenth century German from the Latin root *status* meaning state; originally it meant the study of political facts and figures. The noun random was used in the sixteenth century to mean a haphazard course, from the Germanic randir to run, and as an adjective to mean without a definite aim, rule or method, the opposite of purposive. From the middle of the last century, the concept of a random variable has been used to describe a variable that is a function of the result of a well-defined statistical experiment in which each possible outcome has a definite probability of occurrence. The organization of probabilities of outcomes is achieved by means of a probability function for discrete random variables and by means of a probability density function for continuous random variables. The result of throwing two fair dice and summing what they show is a discrete random variable.

Mainly, we are concerned with continuous random variables (here measurable functions defined on some $\mathbb{R}^n$) with smoothly differentiable probability density measure functions, but we do need also to mention the Poisson distribution for the discrete case.

2

Introduction to Riemannian Geometry

This chapter is intended to help those with little previous exposure to differential geometry by providing a rather informal summary of background for our purposes in the sequel and pointers for those who wish to pursue more geometrical features of the spaces of probability density functions that are our focus in the sequel. In fact, readers who are comfortable with doing calculations of curves and their arc length on surfaces in $\mathbb{R}^3$ could omit this chapter at a first reading.

A topological space is the least structure that can support arguments concerning continuity and limits; our first experiences of such analytic properties is usually with the spaces $\mathbb{R}$ and $\mathbb{R}^n$. A manifold is the least structure that can support arguments concerning differentiability and tangents–that is, calculus. Our prototype manifold is the set of points we call Euclidean n-space $\mathbb{E}^n$ which is based on the real number n-space $\mathbb{R}^n$ and carries the Pythagorean distance structure. Our common experience is that a 2-dimensional Euclidean space can be embedded in $\mathbb{E}^3$, (or $\mathbb{R}^3$) as can curves and surfaces. Riemannian geometry generalizes the Euclidean geometry of surfaces to higher dimensions by handling the intrinsic properties like distances, angles and curvature independently of any environing simpler space.

We need rather little geometry of Riemannian manifolds in order to provide background for the concepts of information geometry. Dodson and Poston [70] give an introductory treatment with many examples, Spivak [194, 195] provides a six-volume treatise on Riemannian geometry while Gray [99] gave very detailed descriptions and computer algebraic procedures using *Mathematica* [215] for calculating and graphically representing most named curves and surfaces in Euclidean $\mathbb{E}^3$ and code for numerical solution of geodesic equations.

3

Information Geometry

We use the term information geometry to cover those topics concerning the use of the Fisher information matrix to define a Riemannian metric, on smooth spaces of parametric statistical models, that is, on smooth spaces of probability density functions. Amari [8, 9], Amari and Nagaoka [11], Barndorff-Nielsen and Cox [20], Kass and Vos [113] and Murray and Rice [153] provide modern accounts of the differential geometry that arises from the Fisher information metric and its relation to asymptotic inference. The Introduction by R.E. Kass in [9] provided a good summary of the background and role of information geometry in mathematical statistics. In the present monograph, we use Riemannian geometric properties of various families of probability density functions in order to obtain representations of practical situations that involve statistical models.

It has by many experts been argued that the information geometric approach may not add significantly to the understanding of the theory of parametric statistical models, and this we acknowledge. Nevertheless, we are of the opinion that there is benefit for those involved with practical modelling if essential qualitative features that are common across a wide range of applications can be presented in a way that allows geometrical tools to measure distances between and lengths along trajectories through perturbations of models of relevance. Historically, the richness of operations and structure in geometry has had a powerful influence on physics and those applications suggested new geometrical developments or methodologies; indeed, from molecular biology some years ago, the behaviour of certain enzymes in DNA manipulation led to the identification of useful geometrical operators. What we offer here is some elementary geometry to display the features common, and of most significance, to a wide range of typical statistical models for real processes.

4

Information Geometry of Bivariate Families

From the study by Arwini [13], we provide information geometry, including the α-geometry, of several important families of bivariate probability density functions. They have marginal density functions that are gamma density functions, exponential density functions and Gaussian density functions. These are used for applications in the sequel, when we have two random variables that have non-zero covariance—such as will arise for a coupled pair of random processes.

The multivariate Gaussian is well-known and its information geometry has been reported before [183, 189]; our recent work has contributed the bivariate Gaussian α-geometry. Surprisingly, it is very difficult to construct a bivariate exponential distribution, or for that matter a bivariate Poisson distribution that has tractable information geometry. However we have calculated the case of the Freund bivariate mixture exponential distribution [89]. The only bivariate gamma distribution for which we have found the information geometry tractable is the McKay case [146] which is restricted to positive covariance, and we begin with this.

5

Neighbourhoods of Poisson Randomness, Independence, and Uniformity

As we have mentioned before, colloquially in applications, it is very common to encounter the usage of ‘random’ to mean the specific case of a Poisson process process whereas formally in statistics, the term random has a more general meaning: probabilistic, that is dependent on random variables. When we speak of neighbourhoods of randomness we shall mean neighbourhoods of a Poisson process and then the neighbourhoods contain perturbations of the Poisson process. Similarly, we consider processes that are perturbations of a process controlled by a uniform distribution on a finite interval, yielding neighbourhoods of uniformity. The third situation of interest is when we have a bivariate process controlled by independent exponential, gamma or Gaussian distributions; then perturbations are contained in neighbourhoods of independence. These neighbourhoods all have well-defined metric structures determined by information theoretic maximum likelihood methods. This allows trajectories in the space of processes, commonly arising in practice by altering input conditions, to be studied unambiguously with geometric tools and to present a background on which to describe the output features of interest of processes and products during changes.

The results here augment our information geometric measures for distances in smooth spaces of probability density functions, by providing explicit geometric representations with distance measures of neighbourhoods for each of these important states of statistical processes:

- (Poisson) randomness,
- independence,
- uniformity.

6

Cosmological Voids and Galactic Clustering

For a general account of large-scale structures in the universe, see, for example, Peebles [162] and Fairall [82], the latter providing a comprehensive atlas. See also Cappi et al [39], Coles [42], Labini et al. [128, 129], Vogeley et al. [208] and van der Weygaert [202] for further recent discussion of large structures. The Las Campanas Redshift Survey was a deep survey, providing some 26,000 data points in a slice out to $500\,h^{-1}Mpc$. Doroshkevich et al. [79] (cf. also Fairall [82] and his Figure 5.5) revealed a rich texture of filaments, clusters and voids and suggested that it resembled a composite of three Poisson processes, consisting of sheets and filaments:

- **Superlarge-scale sheets:**
  60 percent of galaxies, characteristic separation about $77\,h^{-1}Mpc$
- **Rich filaments:**
  20 percent of galaxies, characteristic separation about $30\,h^{-1}Mpc$
- **Sparse filaments:**
  20 percent of galaxies, characteristic separation about $13\,h^{-1}Mpc$.

Most recently, the data from the 2-degree field Galaxy Redshift Survey (2dF-GRS), cf Croton et al. [49, 50] can provide improved statistics of counts in cells and void volumes.

In this chapter we outline some methods whereby such statistical properties may be viewed in an information geometric way. First we look at Poisson processes of extended objects then at coupled processes that relate void and density statistics, somewhat heuristically but intended to reveal the way the information geometry can be used to represent such near-Poisson spatial processes. The applications to cosmology here are based on the publications [63, 62, 64, 65].

7

Amino Acid Clustering

With A.J. Doig

In molecular biology a fundamental problem is that of relating functional effects to structural features of the arrangement of amino acids in protein chains. Clearly, there are some features that have localized deterministic origin from the geometrical organization of the helices; other features seem to be of a more stochastic character with a degree of stability persisting over long sequences that approximates to stationarity. These latter features were the subject of our recent study [34], which we outline in this chapter. We make use of gamma distributions to model the spacings between occurrences of each amino acid; this is an approximation because the molecular process is of course discrete. However, the long protein chains and the large amount of data lead us to believe that the approximation is justified, particularly in light of the clear qualitative features of our results.

7.1 Spacings of Amino Acids

We analysed for each of the 20 amino acids X the statistics of spacings between consecutive occurrences of X within the *Saccharomyces cerevisiae* genome, which has been well characterised elsewhere [95]. These occurrences of amino acids may exhibit near Poisson random, clustered or smoothed out behaviour, like 1-dimensional spatial statistical processes along the protein chain. If amino acids are distributed independently and with uniform probability within a sequence then they follow a Poisson process and a histogram of the number of observations of each gap size would asymptotically follow a negative exponential distribution. The question that arises then is how 20 different approximately Poisson processes constrained in finite intervals be arranged along a protein. We used differential geometric methods to quantify information on sequencing structures of amino acids and groups of amino acids, via the sequences of intervals between their occurrences.

8

Cryptographic Attacks and Signal Clustering

Typical public-key encryption methods involve variations on the RSA procedure devised by Rivest, Shamir and Adleman [174]. This employs modular arithmetic with a very large modulus in the following manner. We compute

$$R \equiv y^e \ (mod\, m) \quad \text{or} \quad R \equiv y^d \ (mod\, m) \tag{8.1}$$

depending respectively on whether we are encoding or decoding a message y. The (very large) modulus m and the encryption key e are made public; the decryption key d is kept private. The modulus m is chosen to be the product of two large prime numbers p, q which are also kept secret and we choose d, e such that

$$ed \equiv 1 \ (mod\, (p-1)(q-1)). \tag{8.2}$$

8.1 Cryptographic Attacks

It is evident that both encoding and decoding will involve repeated exponentiation procedures. Then, some knowledge of the design of an implementation and information on the timing or power consumption during the various stages could yield clues to the decryption key d. Canvel and Dodson [38, 37] have shown how timing analyses of the modular exponentiation algorithm quickly reveal the private key, regardless of its length. In principle, an incorporation of obscuring procedures could mask the timing information but that may not be straightforward for some devices. Nevertheless, it is important to be able to assess departures from Poisson randomness of underlying or overlying procedures that are inherent in devices used for encryption or decryption and here we outline some information geometric methods to add to the standard tests [179].

9

Stochastic Fibre Networks

With W.W. Sampson

There is considerable interest in the materials science community in the structure of stochastic fibrous materials and the influence of structure on their mechanical, optical and transport properties. We have common experience of such materials in the form of paper, filters, insulating layers and supporting matrices for composites. The reference model for such stochastic fibre networks is the 2-dimensional array of line segments with centres following a Poisson process in the plane and axis orientations following a uniform process; that structure is commonly called a *random fibre network* and we study this before considering departures from it.

A classical reference structure for modelling is an isotropic planar network of infinite random lines. So the angles of lines relative to a given fixed direction are uniformly distributed and on each line the locations of the intersections with other lines in the network form a Poisson point process.

The polygons generated by the intersections of lines have been studied by many workers and several analytic results are known. There are results of Miles [147, 148] and Tanner [198] (cf. also Stoyan et al. [196]) for random lines in a plane, for example:

- Expected number of sides per polygon

$$\bar{n} = 4.$$

- Variance of the number of sides per polygon

$$\sigma^2(n) = \frac{\pi^2 + 24}{2}.$$

10

Stochastic Porous Media and Hydrology

With J. Scharcanski and S. Felipussi

Stochastic porous media arise naturally in many situations; the common feature is a spatial statistical process of extended objects, such as voids distributed in a solid or a connected matrix of distributed solids in air. We have modelled real examples above of cosmological voids among stochastic galactic clusters and at the other extreme of scale are the inter-fibre voids in stochastic fibrous networks. The main context in the present chapter is that of voids in agricultural soils.

10.1 Hydrological Modelling

Yue et al. [216] reviewed various bivariate distributions that are constructed from gamma marginals and concluded that such bigamma distribution models will be useful in hydrology. Here we study the application of the McKay bivariate gamma distribution, which has positive covariance, to model the joint probability distribution of adjacent void and capillary sizes in soils. In this context we compare the discriminating power of an information theoretic metric with two classical distance functions in the space of probability distributions. We believe that similar methods may be applicable elsewhere in hydrology, to characterize stochastic structures of porous media and to model correlated flow variables. Phien [166] considered the distribution of the storage capacity of reservoirs with gamma inflows that are either independent or first-order autoregressive and our methods may have relevance in modelling and quantifying correlated inflow processes. Govindaraju and Kavvas [98] used gamma or Gaussian distributions to model rill depth and width at different spatial locations and again an information geometric approach using a bivariate gamma or Gaussian model may be useful in further probing the joint behavior of these rill geometry variables.

11

Quantum Chaology

This chapter, based on Dodson [66], is somewhat speculative in that it is clear that gamma distributions do not precisely model the analytic systems discussed here, but some features may be useful in studies of qualitative generic properties in applications to data from real systems which manifestly seem to exhibit behaviour reminiscent of near-random processes. Quantum counterparts of certain simple classical systems can exhibit chaotic behaviour through the statistics of their energy levels and the irregular spectra of chaotic systems are modelled by eigenvalues of infinite random matrices. We use known bounds on the distribution function for eigenvalue spacings for the Gaussian orthogonal ensemble (GOE) of infinite random real symmetric matrices and show that gamma distributions, which have the important uniqueness property Theorem 11.1, can yield an approximation to the GOE distribution.

Theorem 11.1 (Hwang and Hu [106]). *For independent positive random variables with a common probability density function f, having independence of the sample mean and the sample coefficient of variation is equivalent to f being the gamma distribution.*

This has the advantage that then both chaotic and non chaotic cases fit in the information geometric framework of the manifold of gamma distributions. Additionally, gamma distributions give approximations, to eigenvalue spacings for the Gaussian unitary ensemble (GUE) of infinite random hermitian matrices and for the Gaussian symplectic ensemble (GSE) of infinite random hermitian matrices with real quaternionic elements. Interestingly, the spacing distribution between zeros of the Riemann zeta function is approximated by the GUE distribution, and we investigate the stationarity of the coefficient of variation of the numerical data with respect to location and sample size. The review by Deift [52] illustrates how random matrix theory has significant links to a wide range of mathematical problems in the theory of functions as well as to mathematical physics.

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