

Report No. 7/2002

Stochastic Geometry, Spatial Statistics and Statistical Physics

February 10th – February 16th, 2002

The meeting was organised by A. Baddeley (Crawley), D. Stoyan (Freiberg) and W. Weil (Karlsruhe). During the five days of the conference, 35 talks were given, 15 longer and 20 shorter; additionally, three informal seminars were organized and a poster session. The 47 participants came from Germany (# 26), Australia (# 3), Great Britain (# 3), Czech Republic (# 2), Denmark (# 2), France (# 2), Spain (# 2), USA (# 2), Italy, Hong Kong, Japan, Netherlands and Poland.

The aim of the conference was to present to newest developments in the fields of stochastic geometry and geometry-related spatial statistics and to discuss geometrically oriented work in statistical physics. Thus the participants came from the three areas mathematics, statistics and physics. The interdisciplinary concept of the conference turned out to be very successful; because of the different languages and cultures of the three fields a large number of talks was necessary. The conference was characterized by intensive open discussions between geometers, statisticians and physicists, which have lead to intensified cooperation and new insights and research projects.

The organizers and participants thank the “Mathematisches Forschungsinstitut Oberwolfach” to make the conference possible in the usual comfortable and inspiring setting. The abstracts follow in alphabetical order.

Abstracts

On Quantum Statistical Inference

OLE E. BARNDORFF-NIELSEN

An introductory survey of quantum statistical inference, with emphasis on recent developments, was given. After reviewing the quantum physical rules for determining the probability laws of observational outcomes and the associated key concept of quantum instruments, a number of basic inferential concepts were discussed some of which, but not all, have a classical counterpart. Among these concepts are quantum Fisher information, quantum sufficiency and quantum cuts, quantum exponential models and quantum transformation models, and exhaustivity. Part of the theory was illustrated by a spin-1/2 example, and the fact that classical Fisher information and related asymptotic inference procedures has a central role also in quantum statistics was underlined.

Recent applications of mark correlation functions

CLAUS BEISBART

(joint work with Martin Kerscher (München) and Klaus R. Mecke (Stuttgart))

Marked point processes provide a useful framework to characterize and to model the spatial distribution of objects jointly with their intrinsic properties, called marks. A prominent example is the distribution of galaxies in the Universe with their luminosities or morphological types as marks. One important line of interest in this case is whether the clustering of galaxies depends on their physical properties (“mark segregation”).

After a short introduction into the theory of marked point processes we clarify the notion of mark segregation; introducing mark locality, we distinguish between strong and weak mark segregation. We discuss how commonly known test quantities distinguish between the different levels of mark segregation. In a second step we apply the test quantities to a number of data sets. We find that in the Southern Sky Redshift Survey 2, the luminous galaxies cluster more strongly than the dim ones. The orientations of dark matter halos forming in cosmological N-body simulations show significant alignments. Also, the distribution of Martian craters and holes in a sandstone are investigated with mark correlation functions.

In order to capture some of the empirically found mark correlations quantitatively, we discuss a number of models. Mark segregation can originate from points tracing an independent random field. For galaxies however, this model is not realistic, since galaxies together with their luminosities are not mark-local, contrary to the random field model. A generalization, however, the Cox random field model, can at least qualitatively account for the observed correlations. In order to understand some aspects of Martian craters and holes in a sandstone, we introduce a Boolean depletion model.

Stereology of extremes

VICTOR BENEŠ

(joint work with D. Hlubinka (Prague))

In the stereological unfolding problem for spheroidal particles the aim is to predict extremal shape factor from the observation of extremal shape factor of particle sections. Both marginal and conditional shape factor distribution (given particle size) is investigated by means of the statistical extreme value theory. The stability of stereological transformation with respect to belonging to a given domain of attraction is used to the evaluation of both planar and spatial normalizing constants of some parametric models. This enables prediction of extremal characteristics from real data.

Monte Carlo simulation: A tool of statistical physics to study phase transitions

KURT BINDER

Phase transitions, such as the freezing of water into ice, are very common phenomena in nature. Nevertheless, their theoretical understanding within the framework of statistical thermodynamics is very difficult: one needs to compute the partition function of N interacting particles in the “thermodynamic limit” ($N \rightarrow \infty$) and analyze the resulting singularities.

Monte Carlo simulation provides a tool to solve this problem numerically, and to obtain results that are “exact” apart from numerical errors. At critical points, such as the Curie temperature of an Ising model, where the spontaneous magnetization vanishes, this approach relies on the concept of “finite size scaling”, which allows to carry out the extrapolation ($N \rightarrow \infty$) using a sequence of finite values for N . Nevertheless, there are still simple but important problems such as the freezing transition of the two-dimensional hard disk model fluid, where the answers are inconclusive due to numerical difficulties. The “state of the art” in the treatment of these problems will be reviewed.

The stochastic geometry of the crystallization process of polymers

VINCENZO CAPASSO

Crystallization of polymers is composed of two processes, nucleation (birth) and subsequent growth of crystallites, which are in general both stochastic in time and space. If we assume that at points of contact between two growing crystallites they stop growing, a random division of the relevant region in a d -dimensional space is obtained, known as a random Johnson-Mehl tessellation. The coupling of the kinetic parameters of the birth-and-growth process with the underlying temperature field induces time and space heterogeneities (and stochasticity) of all parameters involved, thus motivating a more general analysis of the stochastic geometry of the crystallization process. A full characterization of the final spatial structure of the crystallization (tessellation) can be given in terms of the mean densities of interfaces (n -facets: cells, faces, edges, vertices) of the random tessellation, at all different Hausdorff dimensions, with respect to the usual d -dimensional Lebesgue measure. It is well known that mechanical properties of the final material strongly depend on the mean densities mentioned above.

Based on a multiple scale approach, evolution equations of the above quantities in terms of the kinetic parameters of the process have been derived, coupled with the evolution equations of the underlying temperature field.

Johnson–Mehl Tessellations: Asymptotics and Inference

SUNG NOK CHIU

(joint work with Ilya Molchanov (Glasgow) and Malcolm Quine (Sydney))

Consider a set of distinct, isolated points, called *seeds*, in a continuous space. A seed at x_i will be stimulated after a time t_i . A seed, once stimulated, immediately tries to germinate and at the same time to prohibit other seeds from germination by generating a spherical inhibited region the radius of which grows at a positive speed v . A seed stimulated at time t_i fails to germinate if and only if its location has been inhibited on or before t_i . The set of locations first inhibited by the growth of the inhibited region originated from x_i is called the cell of x_i . The space will be partitioned into cells and this space-filling structure is called the Johnson–Mehl tessellation.

In this talk we consider the distribution of the time until the cube $[0, L]^d$ is totally inhibited. It has an extreme value distribution, provided that seed locations and stimulation times form a spatially homogeneous Poisson process in $\mathbb{R}^d \times [0, \infty)$. In particular, for $d = 1$, we explain how to obtain the exact distribution of this time by transforming the original process to a Markov process. Moreover, we discuss the number of germinations within $[0, L]^d$. A central limit theorem for this number is shown for the case that seed locations and stimulation times form a Poisson process and then extended to the case that the seed locations are m -dependent.

The second part of the talk is devoted to the estimation of the speed v and the intensity measure (on the time axis) of the Poisson process. The maximum likelihood estimation for v , a nonparametric estimation for the intensity measure and for its density, and the maximum likelihood estimation for the parameters of the intensity with known analytical form are proposed and applied to real neurobiological data.

Pseudosystematic sampling on the sphere

LUIS M. CRUZ-ORIVE

(joint work with Ximo Gual-Arnau (Castellón))

In geometric sampling, and local stereology in particular, it is often required to estimate an integral of the form:

$$Q = \int_{\mathbb{S}^2} f \, d\omega = \int_0^{2\pi} \int_0^\pi f(\phi, \theta) \sin \theta \, d\theta \, d\phi$$

where $f : \mathbb{S}^2 \rightarrow \mathbb{R}^+$ is a non random function defined on the unit sphere \mathbb{S}^2 and square integrable on it. For instance, if Q represents the volume of a bounded particle which is star convex with respect to the origin and $r(\phi, \theta)$ is the length of the radius vector of the particle in the direction (ϕ, θ) , then $f(\phi, \theta) = (1/3) r^3(\phi, \theta)$. To estimate Q , some sort of systematic design on \mathbb{S}^2 becomes necessary on grounds of efficiency and practical applicability. Typically the relevant probes are of nucleator type, in which several rays emanate from a fixed origin, (e.g. from a nucleolus within a biological cell), and they are contained in a sectioning plane through the origin. The latter requirement considerably

reduces the choice of design in practice. Here we concentrate on a nucleator design based on splitting the sphere into regions of equal area, but not of identical shape; the design is therefore 'pseudosystematic'. First we present a useful exact representation of the variance of an unbiased estimator of Q under the mentioned design. Then we adopt a suitable covariogram model to obtain a variance predictor from a single sample of arbitrary size, and finally we examine the prediction accuracy by way of simulation on a synthetic particle model.

Surface shape analysis from MR images

IAN DRYDEN

Statistical shape analysis is of interest in a variety of applications. Although many applications have been landmark-based, there is a growing number of examples where shapes of curves and surfaces are investigated. We restrict ourselves to star-shaped objects which can be represented by a radial function on a sphere, or a subset of the sphere. We initially consider a Bayesian method for registration to the midline by translation and rotation using symmetry properties of the midline neighborhood. Samples from the posterior are obtained using a Markov chain Monte Carlo algorithm. By conditioning on the registration, size and shape inference can be carried out by adapting the tools of functional data analysis. The method is applied to a dataset of MR images investigating large scale structure of the brain of schizophrenia patients, which is joint work with Antonio Gattone (University of Chieti, Italy), Bert Park and Stuart Leask (Nottingham) and Sean Flynn (University of British Columbia).

Random geometry of the two-dimensional Ising model

HANS-OTTO GEORGI

For various lattice systems of interacting spins, the phenomenon of phase transition goes parallel with the presence of infinite percolation clusters. This holds in particular for the classical Ising model of ferromagnetism. We show that in this model the percolation picture also provides information on the number of phases: There exist only two distinct phases if and only if there is no coexistence of infinite plus- and minus-clusters, and this is the case for a number of planar lattices including \mathbb{Z}^2 . This result extends and simplifies a famous theorem of Russo-Aizenman-Higuchi (1980) and is based on various geometric ideas together with the use of a spatial strong Markov property and stochastic domination techniques.

Locally scaled point processes

UTE HAHN

Point patterns observed in nature are often inhomogeneous due to inhomogeneity of the substrate bearing the pattern. In many such cases, regions with different intensity appear to be realizations of the same point process up to a scale factor.

An approach will be presented to defining models for such inhomogeneous point processes by modifying the density function of a homogenous template process. To this end, the volume measures occurring in the definition of the template density are replaced with so called locally scaled volume measures. These volume measures are defined with respect to

a location dependent scaling function. If the scaling function is constant, then local scaling coincides with global scaling by a constant factor. The proposed method can principally be applied to any homogeneous template point process that has a scale invariant density with respect to the Poisson point process, thus leading to a wealth of possible models.

It will also be discussed how statistics for stationary point processes such as the nearest neighbour distance distribution or the empty space function carry over to the locally scaled case.

Asymptotic Normality of the Euler - Poincaré Characteristic of Boolean Models in Large Sampling Windows

LOTHAR HEINRICH

Having in mind Hadwiger's recursive definition of the Euler-Poincaré-characteristic (E-P-C) for sets in the convex ring we introduce the point processes Ψ_u^+ and Ψ_u^- of exposed positive resp. negative tangent points in direction $u \in S^1$ associated with a planar germ-grain model $\Xi = \cup_{i \geq 1} (\Xi_i + X_i)$, where $(\Xi_i)_{i \geq 1}$ are i.i.d. random convex, compact sets being independent of the point process $\Psi = \sum_{i \geq 1} \delta_{X_i}$. According to the well-known *tangent count method* used in stereology we define the empirical mean E-C-P $\hat{N}_{A,n}(u)$ (in direction $u \in S^1$) as ratio of the difference $\Psi_u^+(W_n) - \Psi_u^-(W_n)$ and the area $|W_n|$ of the rectangular, unboundedly expanding sampling window W_n . We prove strong consistency for this unbiased estimator of N_A for stationary ergodic second-order point processes Ψ . For Poisson-grain models we derive a CLT under mild conditions on the primary grain. In case of strictly bounded grains a consistent estimation of the asymptotic variance, Berry-Esseen bounds and Edgeworth expansions in the local CLT are presented. These results are based on corresponding advanced limit theorems for m -dependent random fields. Analogous results are possible in the $3D$ - case.

Carbon clusters and clusters of carbon clusters

HELMUT HERRMANN

(joint work with F. Fugaciu and A. Touzik)

Carbon can form a great variety of ordered, partially ordered and random networks realized in 3D space, on parallel flat planes, and on corrugated planes of finite size. The reason for this is that the four electrons of the valence shell of the carbon atoms can arrange to different stable hybridization states. Therefore, carbon atoms can switch between two chemical bonds, i.e. two neighbours, three bonds (trigonal planar symmetry), and four bonds (tetrahedral symmetry). We used molecular dynamics (see contribution by U. Rößler) and a density-functional based method for the calculation of the interatomic forces and studied the transformation of graphitic and diamond-like particles into other types of particles. The simulations were carried out at temperatures between 1500K and 2800K. Additionally, a random process was included modelling irradiation effects. The shape of the particles obtained and the topology of the network of atoms ranged from fullerenes (regular arrangement of pentagonal and hexagonal cells on a sphere), continuous random networks arranged on spherical or drop-like surfaces and on corrugated planes of finite size, concentric-shell fullerenes interconnected by atoms with four bonds, and spiraloidal particles. Some of these particles have not been observed in nature until now. We showed empirically that (with limited reliability) it is possible to predict the type of the final

particle from the simulation conditions. During most of the simulations the intermediate structure developed after few thousands of time steps was similar to a 3D continuous random network. It is, however, not clear which properties of these networks control the evolution of the system and decide about the type of the final particle obtained after 50.000 to 100.000 time steps. Fullerenes can be deposited on a substrate. The fullerenes are then situated on the nodes of a crystalline face-centred cubic lattice. Adding potassium atoms to the fullerene layer the surface morphology of the fullerene film changes its character. From the initial surface which is smooth on a molecular scale, a system of random but densely arranged hillocks develops on a 20nm to 50nm scale. We tried to find out the physical reason for this transformation using a kinetic Monte Carlo method (see contribution by K. Binder). A box consisting of a face-centred cubic lattice with about 1 million of fullerene molecules was considered where periodic boundary conditions in two direction were applied simulating thin films of either 64 or 128 fullerene diameters in thickness. Potassium atoms were distributed at random on the tetrahedral and octahedral holes of the lattice. The number of potassium atoms was between 5% and 30% of the number of fullerene molecules. It turned out that electrostatic forces and repulsive interactions of the electron shells of the fullerenes are responsible for the structural changes. The simulations reproduced the mean size of the hillocks. Additionally, we showed that the potassium concentration in the hillocks has a stoichiometric value pointing to the formation of a special potassium fulleride phase. This phase has metallic character. Therefore, the decomposed fulleride layer can, e.g., be used as an array of nanometre-scale electrodes for electrochemical applications.

Stochastic modelling of particle sedimentation in fluids

CHRISTIAN H. HESSE

The talk starts by reviewing some non-stochastic approaches to the problem of modelling particle sedimentation in fluids. It then presents a stochastic model based on coupled Ornstein-Uhlenbeck processes whose parameters depend on system-configuration. Various aspects including model structure, model dynamics, model fitting and support for the model are discussed in detail.

Micro-Macro-Transition for Transport in Porous Media

RUDOLF HILFER

The talk discusses the problem of transport (e.g. fluid flow or electrical conduction) through macroscopically and microscopically heterogeneous porous media. The porous medium is assumed to be a discretized random set. Realizations are given as three-dimensional computer tomographic images. Fluid flow is described by Stokes equations with no-slip boundary conditions on the microscopic pore scale l . It is known that in the macroscopic limit $\varepsilon = \frac{l}{L} \rightarrow 0$, the fluid flow is described by Darcy's equation with permeability $k(\varepsilon)$ where l is the typical pore size and L is the system size. Assuming that the porous medium is macroscopically homogeneous (stationary, ergodic), it is generally believed that for fixed $\delta > 0$ there exists an ε^* such that $k(0) - \delta < k(\varepsilon) < k(0) + \delta$ for all $\varepsilon^* > \varepsilon$. The talk focusses on two questions: i) What is the numerical value of ε^* ? ii) Can ε^* (and in fact $k(\varepsilon)$) be calculated approximately from purely geometric functionals of the porous medium? First the microscopic equations are solved numerically using two methods: finite difference techniques and lattice-Boltzmann simulations. The results are found to be slightly different and to depend on discretization. Secondly the results are

compared to a generalized self-consistent effective medium theory introduced earlier under the name “local porosity theory” (Phys. Rev. B **44**, 60 (1991), Phys. Rev. B **45**, 7115 (1992), Adv. Chem. Phys. **XCII**, 299 (1996)). Local porosity (geometry) distributions were introduced there as empirical histograms of Minkowski functionals measured in a cell of size L . Local porosity distributions and local percolation probabilities provide geometric descriptors that depend explicitly on length scale and lead to approximate values for k (and other transport properties such as electrical conductivity etc.). A certain integral of both quantities is found to provide an estimate for ε^* that agrees with the exact microscopic calculation not only for permeability k but also for other parameters of physical transport.

Trends in Integral Geometry

DANIEL HUG

A major theme in integral geometry is the study of mean values of functionals of geometric objects. In this talk, we describe several examples of recent results in this direction.

I. Steiner type formulas

We describe a local Steiner type formula for general closed sets in a Euclidean space. Such a formula has first been stated by Stachó in 1979; it seems, however, that the result has been overlooked so far. We present the result in a more modern language, give an explicit description for the associated curvature measures in terms of generalized curvature functions and develop some of the properties of these curvature measures.

II. Translative and kinematic formulas

We then present general integral formulas for curvature measures of \mathcal{U}_{PR} sets (certain locally finite unions of sets with positive reach), due to J. Rataj and M. Zähle (2001), and for the Euler characteristic of convex surfaces (D. Hug, R. Schätzle (2001) and D. Hug, R. Schätzle, P. Mani-Levitska (2002)). The translative results involve different kinds of mixed functionals.

III. Integral geometry of tensor valuations

Finally, we explain some recent translative, kinematic and Crofton formulas for tensor valuations. Such valuations have been suggested as descriptors for spatial patterns, see the recent work of C. Beisbart, R. Dahlke, K. Mecke and H. Wagner (2002). A complete system of integral formulas for tensor valuations is still not available in the literature, partial results, which in particular cover the dimensions two and three, are contained in contributions by R. Schneider (2000) and R. Schneider and R. Schuster (2001).

Change of scale in random sets

DOMINIQUE JEULIN

By image analysis of the microstructure of materials, or by means of models of random sets, it is possible to access to morphological data such as correlation functions, that can be used as an input to predict macroscopic (or effective) physical properties (like the thermal conductivity, the dielectric permittivity, or the elastic moduli) of heterogeneous media.

Bounds of effective properties, depending on limited statistical information, can be obtained from variational principles deduced from the physical problem under study. The most famous bounds are Hashin and Shtrikman bounds, which only depend on the volume fraction of components for a statistically isotropic and stationary random medium. However, many different morphologies can be imagined for given volume fractions. Tighter bounds are obtained after introduction in the variational principles of trial fields depending on the

microscopic properties at different points. For random media with isotropic elastic components and with an isotropic geometry, order three bounds (depending on the 3-points correlation functions) were derived by Beran and Molyneux for the modulus of compressibility K and by McCoy for the shear modulus G . These bounds are valid for multi-component media, and more generally for elastic variables modelled by random functions.

We will illustrate this approach in the case of various two-phase random composites, following the simplifications made Milton. A special construction is obtained for the union or the intersection of multi-scale independent random sets [1]. In the case of two scales, it shows the effect of random clusters on the macroscopic elastic properties. By iteration, optimal multiscale random microstructure, from the point of view of the macroscopic behaviour, are obtained. Finally we will give an introduction to fluctuations of effective properties with the scale of homogenization [2].

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Testing hypothesis that a point process is non-homogeneous Poisson process versus possible dependence structure

ESTATE V. KHMALADZE

The specialists know that to test whether a point process in R^d is some Poisson process, homogeneous or not, against alternative that there is dependence in distribution of points - say, attraction and clustering or repulsion of some sort - is a difficult problem. However, discussion during the conference (with D.Stoyan, A Baddeley, L.Heinrich, I.Molchanov and some other colleagues) helped to realise that methods developed for different purposes, and, namely, so called "scanning martingales", introduced and studied in Khmaladze (1988, 1993) can lead to relatively complete solution of this problem and provide us with the process to base the whole class of statistical tests upon it.

The assumption on intensity of the Poisson process is that it is $n\lambda(\cdot, \theta)$ belongs to some given m -dimensional subspace of functions in R^d (and θ is the vector of its Fourier coefficients). Practically, m can be as high as 10-15.

The approach is to consider the difference between the point process and its intensity measure with estimated parameters and to construct the scanning martingale for it. Then this scanning martingale can be rescaled, using estimated intensity function $\lambda(\cdot, \theta)$, to the process converging in distribution, under hypothesis of Poissonity, to the standard Brownian motion.

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Reconstruction of the Oriented Rose of Normal Directions

MARKUS KIDERLEN

We consider the mean normal measure $\overline{S}(Z, \cdot)$ of a stationary random set Z in the extended convex ring in \mathbb{R}^d . The normalization of this measure, the oriented rose of normal directions, is the distribution of the outer unit normal at a typical boundary point of Z .

It is well known that the family of mean normal measures $\overline{S}'(Z \cap L, \cdot)$ (computed in L) determines $\overline{S}(Z, \cdot)$ uniquely, if L runs through all k -dimensional linear subspaces for some fixed $k \in \{2, 3, \dots, d-1\}$. It is shown that for $k \neq 2$ this still holds true, even if all the planes L are assumed to belong to a pencil, i.e. contain a given line. For $k = 2$ some mild additional condition is needed. Furthermore, adapting results from discrete Geometric Tomography, we show that the knowledge of $\overline{S}'(Z \cap L, \cdot)$ for a finite number m of k -planes L does not *determine* $\overline{S}(Z, \cdot)$. On the other hand, if $\overline{S}(Z, \cdot)$ has finite support, it can be *verified* from this information (for suitable chosen m).

Finally we suggest a new estimator for $\overline{S}(Z, \cdot)$ in the plane ($d = 2$), based on conditional intersection counts with test lines. The estimator is the solution of a quadratic program and – under some mild conditions on the estimation procedure – is strongly consistent.

Virtual Materials Lab: Imaging and reconstruction, visualising and modelling complex materials

MARK A. KNACKSTEDT

How does a contaminant move through soil? How can we accurately assess a patient's risk of osteoporosis? Why does ink-jet printing give clean sharp lines on some paper, while it smudges on others? Answering these questions require the ability to predict the mechanical and transport properties of complex media from a knowledge of material microstructure. I describe how new experimental techniques are available to image complex materials at a micron scale in 3D. These techniques will greatly impact on our understanding of complex materials. There is an urgent need for a parallel development of expertise in 3D image analysis and morphological characterisation to harness the potential of these 3D imaging methods. This will allow researchers to develop meaningful correlations between morphological measures and physical properties of complex 3D materials.

Contact distributions of Boolean models

GÜNTER LAST

(joint work with Daniel Hug (Freiburg) and Wolfgang Weil (Karlsruhe))

Contact distributions are important characteristics of random closed sets. Their empirical counterparts provide a convenient and useful summary statistics of spatial data. We discuss the basic analytic properties of the contact distributions of a stationary Boolean model first in case of convex grains and then in case of a model with rather general compact grains. We then introduce a general (non stationary) Boolean model and show that all of the previous results can be extended to this case. Finally we indicate some useful generalizations of contact distributions.

Markov sequential spatial processes

MARIE-COLETTE VAN LIESHOUT

A simple sequential inhibition point process (SSI) is defined as the output of an algorithm that repeatedly introduces particles at random into a bounded window, discarding those that would overlap a previously introduced particle. In this talk, we present ‘Markov sequential spatial processes’, i. e. point patterns that – as SSI – can be imagined to arise as the output of a sequential algorithm and that satisfy a local dependence property, and prove a Hammersley-Clifford style factorisation. Examples other than SSI include local scaling. Cf. (Hahn, Jensen, Van Lieshout, Nielsen; 2001).

Spatial statistics in cosmology

VICENT MARTINEZ

In cosmology, we need to compare the results of the theoretical models of structure formation and the N-body simulations with the real observations of the galaxy distribution. This comparison is mainly performed by means of statistical methods. I have reviewed in this talk the main applications of spatial statistics to the description of the large-scale structure of the universe. Special topics discussed in this talk were: description of the galaxy samples, selection effects and biases, correlation functions, nearest neighbour statistics, Minkowsky functionals, Fourier analysis, and structure statistics. Particular attention have been devoted to the use of scaling laws, fractals, and lacunarity measures in the description of the cosmic texture.

Networks generated by random tessellations

JOSEPH MECKE

A stationary random tessellation in \mathbb{R}^d , i. e. a homogeneous random division of the d -dimensional Euclidean space into bounded convex polytopes, generates the networks (skeletons) N_k , where N_k denotes the union of all closed k -faces ($k = 0, \dots, d$).

The mean connectivity number (mean Euler characteristic per unit volume) of N_k can be expressed as a function of the intensities of j -faces ($j = 0, \dots, k$).

The purpose of the talk is to present a special proof for known results; i. e. for the stochastic counterpart of the well-known Euler-Schläfli-Poncaré formula.

Applications of integral geometry in statistical physics

KLAUS MECKE

The morphology of fractals, dewetting structures and chemical reaction patterns can be described in terms of curvature integrals (Minkowski functionals, which allow a detailed scaling analysis, a comparison of theory and experiment, and the prediction of quantitative physical laws. Integral geometry can also be used to derive Rosenfeld’s density functional theory which give accurate predictions of the structure of inhomogeneous hard body fluids. The application of density functional theory in spatial statistics is emphasized as a general tool to derive generating functionals which might be useful for parameter estimation and inference in Gibbsian systems.

From leaching in soil to coverage in Boolean models

ILYA MOLCHANOV

(joint work with V. Scherbakov (University of Glasgow) and S. Zuyev (University of Strathclyde))

This work is motivated by studies of leaching of bacteria through soils in order to predict the pattern of leaching and chances of bacteria reaching ground water. Assuming that bacteria perform a diffusion through soil, the relevant mathematical model could be Brownian motion in a space with traps. We mention classical results in this area and highlight special effects that appear when dealing with the trapping problem for the Wiener process with the time added as an additional component.

The experiments show however that the leaching properties of bacteria at the first approximation resemble those of inert colloidal particles. The bacteria move when the soil is sufficiently wet, and if they hit a dry patch of soil at a certain depth, then the bacteria die. This suggests a model for bacteria transport that concentrates on macro properties of soil and so allows for transparent mathematical formulation in the language of semi-linear processes. The main result concerns finding probabilities of bacteria moving through and the explicit expression for the critical function that describes the (inhomogeneous) speed of bacteria ensuring that they die eventually with probability one. It is shown how this problem is related to the ruin problem in insurance and to the studies of the exponential integrals of stochastic processes. The multidimensional variants of this problem would correspond to finding conditions under which the whole plain is covered by an inhomogeneous Boolean model. The corresponding critical function is also given.

Perfect simulation and inference for spatial point processes

JESPER MØLLER

(joint work with Kasper K. Berthelsen (Aalborg))

The advantages and limitations of using perfect simulation for simulation-based inference for pairwise interaction point processes are discussed. Various aspects of likelihood inference for the Strauss process with unknown range of interaction are studied. A large part of the talk concerns non-parametric Bayesian inference for the interaction function. Markov chain Monte Carlo methods, particularly path sampling, play an important role. Several empirical results and various datasets are considered.

Limits of sequences of stationary planar tessellations, generated by iterated superposition and nesting

WERNER NAGEL

(joint work with Viola Weiss (Jena))

In order to increase the variety of feasible models for random stationary tessellations (mosaics) two operations acting on tessellations are studied: superposition and nesting (the latter is also referred to as iteration). The superposition of two planar tessellations means the superposition of the edges of the cells of both tessellations. This generates a new tessellation where the cells are intersections of pairs of cells of the original tessellations. The iteration of tessellations is a more sophisticated operation. It means that one tessellation is chosen as a 'frame' tessellation. The single cells of this 'frame' tessellation

are consecutively and *independently* subdivided by cut-outs of tessellations of an i.i.d. sequence of tessellations. Thus different cells of the 'frame' tessellation are intersected with different realisations of other tessellations.

In the lecture, for sequences of tessellations which are generated by iterated application of superposition or iterated nesting respectively, the limits are investigated.

Sequences of (renormalised) superpositions of stationary planar tessellations converge weakly to Poisson line tessellations.

For an iterated nesting the notion of stability of a distribution is adapted and necessary conditions are formulated for those tessellations which may occur as limits.

Tessellation-based hierarchical modelling of space-time earthquake occurrences

YOSHIKO OGATA

My talk is concerned with modelling and analysis of earthquake data of occurrence times, locations ignoring depth, and magnitudes. A space-time point-process model is specified in which earthquake intensity is modelled as a function of previous activity. Specific forms of the function of locations and times are based on the established empirical laws in seismology, but their parameters are known to be different from place to place. Thus each parameter is function of location (but not time) represented by linear interpolation over Delaunay tessellation based on observed locations of earthquakes. Using a smoothness constraint for each parameter in the model, a penalised likelihood method is considered for fitting, where the optimal weights of the penalties are objectively tuned by an empirical Bayesian method.

Having done that, my final goal is to measure the temporal deviation of the actual seismicity rate from that of the predicted occurrence rate by the estimated model. For this procedure I considered space-time smooth functions represented by linear interpolation over a 3-dimensional tessellation based on observed times and locations of earthquakes, and carry out the similar penalised likelihood method as the above procedure. There are a number of zones where temporal deviation from the fitted model, with quiet periods (relative quiescence), took place before large earthquakes.

I also presented statistical evidence that, after relative quiescence in the aftershock activity, a significantly higher probability of a large event is expected in the neighbourhood (say, within 200km radius) during the first 6 years, than the case where the aftershocks decayed normally. Further, physical mechanism of the relative quiescence is speculated and illustrated by the aid of the Coulomb's Failure Function assuming a precursory slip in the focal fault.

The Euler number of discretized sets – an appropriate choice of adjacency in homogeneous lattices

JOACHIM OHSER

Two approaches for determining the Euler-Poincaré characteristic of a set observed on lattice points are considered in the context of image analysis – the integral geometric and the polyhedral approach. Information about the set is assumed to be available on lattice points only. In order to retain properties of the Euler number and to provide a good approximation of the true Euler number of the original set in the Euclidean space, the appropriate choice of adjacency in the lattice for the set and its background is crucial.

Adjacencies are defined using tessellations of the whole space into polyhedrons. In \mathbb{R}^3 , two new 14 adjacencies are introduced additionally to the well known 6 and 26 adjacencies. For the Euler number of a set and its complement, a consistency relation holds. Each of the pairs of adjacencies (14.1, 14.1), (14.2, 14.2), (6, 26), and (26, 6) is shown to be a pair of complementary adjacencies with respect to this relation. That is, the approximations of the Euler numbers are consistent if the set and its background (complement) are equipped with this pair of adjacencies. Furthermore, sufficient conditions for the correctness of the approximations of the Euler number are given. The analysis of selected microstructures and a simulation study illustrate how the estimated Euler number depends on the chosen adjacency. It also shows that there is not a uniquely best pair of adjacencies with respect to the estimation of the Euler number of a set in Euclidean space.

The set covariance and its generalizations

JAN RATAJ

Given a nonempty compact subset $X \subseteq \mathbf{R}^d$, the set covariance $\psi_X(u) = \lambda^d(X \cap (X - u))$ is an important characteristic of X used in image analysis (λ^d is the Lebesgue measure). It is well known that the first derivative of ψ_X in direction v at the origin equals minus the measure of the projection of X in direction v , if X is a full-dimensional convex body. We generalize this result to sets X representable as finite unions of sets with positive reach. We also present some particular results on the information contained in the higher order derivatives at the origin of ψ_X for smooth convex bodies X .

Gauge invariance in two-dimensional foam

NICOLAS RIVIER

(joint work with C. Oguey (Cergy-Pontoise) and T. Aste (Canberra))

Two-dimensional foams are random tilings by topological polygons. The only random variable is the number n of sides of a cell (topological charge $6-n$). Tilings are homogeneous overall, and globally invariant under local topological transformations, i.e. gauge invariant. Gauge invariance yields, through maximum entropy, the mark distribution (of an n - and a k -sided cells at a topological distance j) and an asymptotically unique distribution pn . A Gauss theorem relates the flux of edges through a closed contour to the total topological charge within. By differentiation, one obtains a stratification of the foam into parallel layers, which roughen in a controlled fashion. The foam is tiled by square plaquettes, which are the intersection of two layers in the two, “orthogonal” stratifications. The plaquettes are frustrated if they contain more than one cell. Frustrated plaquettes serve as a local “order parameter” for disorder.

Molecular Dynamics Simulations of Metallic Glasses: Chemical Fluctuations and Polyamorphous Structures

ULRICH K. RÖSSLER

Metallic Glasses are generally alloys, i.e. multi-component systems, where fluid-like atomic configurations are frozen in a kinetic process that suppresses crystallization. Experimental data indicate ordering phenomena in glassy materials on length scales larger than the short-range order in the corresponding melts. In particular, chemical fluctuations are endemic in these structures. They may appear already in supercooled alloy-melts and may result in a macroscopic decomposition into different amorphous metastable “phases”. Such structures are built by different amorphous packings of atoms in different regions of space. In this talk, results from molecular dynamics simulations on realistic models of metallic glasses for binary and ternary alloy systems showing such effects are presented. A few simple measures and heuristic rules for the analysis of the different amorphous packings found from simulation are introduced. Some more advanced problems of a quantitative description of these complex amorphous structures are discussed: Chemical fluctuations in the equilibrium melts may be analysed as a Gibbs point processes, however, the complete kinetic process leading to glass formation is not an equilibrium process in the sense of statistical physics. Generally, metallic bonds are many-body effects inducing interatomic potentials beyond pair-potentials. Therefore, fluid-like structures for metallic systems should display many-body correlations beyond the usual (partial) pair-correlation functions.

Estimation of the pair correlation function via inverse space

KATJA SCHLADITZ

(joint work with Karsten Koch (Siegen) and Joachim Ohser (Kaiserslautern))

Let Φ be a stationary point process with intensity λ , observed in a compact window W . Denote by $c_W(h) := \text{vol}(W \cap (W - h))$ the window function and by \mathcal{F} the Fourier transform.

The pair correlation function g of Φ can be estimated by

$$\hat{g}(x) = \frac{1}{\lambda^2 c_W(x)} \mathcal{F}^{-1}(|\mathcal{F}((\Phi * \kappa)\mathbf{1}_W)|^2)(x) - \frac{1}{\lambda} \kappa_2(x),$$

where κ is a bounded kernel function with compact support and $\kappa_2 := \kappa * \kappa^*$ with $*$ – convolution and $f^*(x) := f(-x)$.

This new estimator works as good as the usual kernel estimator for g . For large data sets and point process data given as an image, the new estimation procedure can be considerably faster.

Fractal dimension and long memory dependence of random fields

MARTIN SCHLATHER

The Cauchy class provides 2-parameter models for the covariance function that allows for modelling random fields whose graphs have arbitrary fractal dimension and long memory dependence. The Cauchy class has a non-separable extension for space-time modelling. A contributed package for R is presented that allows for ML estimation of the parameters, and provides simulation algorithms.

Iterated Random Tessellations

VOLKER SCHMIDT

(joint work with Roland Maier (Ulm))

The iteration of random tessellations in R^d is considered, where each cell of an initial tessellation is further subdivided into smaller cells by so-called component tessellations. We first show that an iterated tessellation can formally be defined as a point process of closed sets, generated by an initial tessellation and a sequence of component tessellations. Starting, for example, from Poisson-Voronoi tessellations or Poisson hyperplane tessellations, the iteration of tessellations provides a method to construct more general models of random tessellations, which still are tractable from the computational point of view.

Sufficient conditions for stationarity and isotropy of iterated tessellations are given, where we assume in particular that the component tessellations are exchangeable. Furthermore, we show how the intensities of the facet processes of stationary (and isotropic) iterated tessellations can be expressed by quermassintensities of the facet processes of their initial and component tessellations respectively. In connection with this, we consider the notion of an embedded (i, k) -facet process, which consists of those i -facets of the iterated tessellation embedded in k -facets of the initial tessellation; $i \leq k$.

We first derive such intensity formulae for superpositions of tessellations, and then for independent iteration of cells. In the latter case, multiply superimposed component tessellations occur, whose quermassdensities have to be computed recursively. Furthermore, formulae are derived for the expected intrinsic volumes of the typical i -facet of iterated tessellations.

Bernoulli thinning of iterated tessellations is also considered, where only some cells of the initial tessellation are iterated, letting the remaining cells unchanged.

Thermodynamic formalism for asymptotic geometry of set-valued union processes

TOMASZ SCHREIBER

Consider a locally compact and separable metric base space E . A set-valued stochastic process $X^{[t]} \subseteq E$ is called union infinitely divisible iff $X^{[t_1+t_2]}$ coincides in distribution with the union of independent copies of $X^{[t_1]}$ and $X^{[t_2]}$. An important subclass of such processes are those admitting the representation

$$X^{[t]} = \bigcup_{k \leq N_t} X_k,$$

where N_t is a homogeneous Poisson counting process on \mathbb{R} while X_1, X_2, \dots are i.i.d. copies of a certain random set $X \subseteq E$, usually referred to as the grain.

If the grain X is taken *thick* enough, the process $X^{[t]}$ tends to fill the base space E rather fast as $t \rightarrow \infty$. For a fixed normalised measure μ on the base space E , with certain additional conditions we show there exists an exponent $\gamma \in (0, 1)$ with

- $\mathbb{E}\mu(E \setminus X^{[t]}) = \mathbb{E}\mu(X^{[t]^c}) = \Theta(t^{-\gamma})$ and the corresponding strong law of large numbers holds,
- $\text{Var}(\mu(X^{[t]^c})) = \Theta(t^{-\gamma-1})$ and the corresponding central limit theorem holds.

Our purpose is to provide an asymptotic description of the geometry of $X^{[t]}$ for large t . Extremely irregular local behaviour of $X^{[t]}$ and lack of natural affine structure on the family of subsets of the base space E obviate the use of usual normalisation-based asymptotic

analysis procedures. We adopt here a different approach, originating from the area of statistical mechanics. For $\beta > 0$, referred to as the inverse temperature, consider the set-valued process $X^{[t;\beta]}$ defined as the Gibbsian modification of $X^{[t]}$ with Hamiltonian $\beta t\mu(\cdot)$, so that

$$\frac{d\mathcal{L}(X^{[t;\beta]})}{d\mathcal{L}(X^{[t]})}[F] := \frac{\exp(-\beta t\mu(F))}{\mathbb{E} \exp(-\beta t\mu(X^{[t]}))}, \quad F \subseteq E.$$

The modified random set $X^{[t;\beta]}$ has a very natural geometrical interpretation as coinciding in distribution with the law of the original set $X^{[t]}$ conditioned on the event that $X^{[t]} \cap \Pi_{\beta t\mu} = \emptyset$, where $\Pi_{\beta t\mu}$ is a Poisson point process on E with intensity measure $\beta t\mu$, independent of $X^{[t]}$. We show that for small β (high temperature region) the Gibbs process $X^{[t;\beta]}$ represents a small perturbation of $X^{[t]}$ and it shares its strong asymptotic properties. In particular, we have

- $t^{-1}\mathcal{H}(\mathcal{L}(X^{[t;\beta]})|\mathcal{L}(X^{[t]})) = \Theta(t^{-\gamma})$

with \mathcal{H} standing for the usual relative entropy. Moreover, the (renormalised) specific free energy $P(\beta; t) := t^{-1} \log \mathbb{E} \exp(\beta t\mu(X^{[t]^c}))$ decays as $t \rightarrow \infty$ according to the power law $P(\beta; t) = \Theta(t^{-\gamma})$ and, furthermore, we have $\mathbb{E}\mu(X^{[t;\beta]^c}) = \Theta(t^{-\gamma})$ as well. We exploit these facts to derive moderate deviation type results for $\mu(X^{[t]^c})$, stating that

- $\mathbb{P}(|\mu(X^{[t]^c})/\mathbb{E}\mu(X^{[t]^c}) - 1| > \epsilon) \leq \exp(-C(\epsilon)t^{1-\gamma}), \quad \epsilon > 0.$

Some further details about the asymptotic geometry of $X^{[t]}$ are obtained by a more refined high-temperature analysis of the Gibbs processes $X^{[t;\beta]}$.

With increasing β a *phase transition* occurs and for β larger than a certain critical value β_0 (in the low temperature region) the process $X^{[t;\beta]}$ starts to exhibit totally different properties. The volume $\mu(E \setminus X^{[t;\beta]})$ not covered by the Gibbs process does not decay to 0 anymore and the shape of $X^{[t;\beta]}$ is determined by the large deviation principle with speed t and with rate function

- $I_\beta(F) := \beta\mu(F) + T_X(F^c) - \inf_{\hat{F} \subseteq E} [\beta\mu(\hat{F}) + T_X(\hat{F}^c)], \quad F \subseteq E,$

where $T_X(A) := \mathbb{P}(X \cap A \neq \emptyset)$ stands for the hitting functional of the single grain X . Thus, $X^{[t;\beta]}$ has to be asymptotically close to one of the minimisers of I_β . This characterisation is not complete, however, as I_β can happen to admit multiple minimisers. A more detailed analysis of certain specific models (Boolean germ-and-grain models etc) shows that the right asymptotic shape can often be found as minimising a certain model-specific *surface energy* (*surface tension*) and it coincides with an appropriate convex body referred to as *Wulff crystal* in the language of statistical mechanics. A detailed analysis of the low-temperature behaviour of $X^{[t;\beta]}$ yields some further large deviation type results for $X^{[t]}$.

We conclude our talk with an example application of the developed methods to certain classical problems of stochastic geometry. In particular, we suggest a new approach to the asymptotic analysis of convex hulls generated by high-intensity Poisson point processes in a multidimensional ball. The results obtained in this way include appropriate large deviation principles, central limit theorems and strong laws of large numbers which are valid in arbitrary dimension. We compare these results with the rich existing literature of the subject.

Fluid Membranes

UDO SEIFERT

Fluid membranes are closed two-dimensional surfaces embedded in three-dimensional space. These so-called vesicles form spontaneously when lipid molecules are dissolved in aqueous solution. The large variety of observed shapes can be derived from a simple variational principle. These shapes are minima of the curvature energy which is given by the integral of the squared mean curvature over the whole shape. While naive minimization leads to a sphere, the physical boundary conditions of fixed volume, area and total mean curvature render this problem non-trivial.

For higher topology the conformal invariance of this energy leads to a degeneracy of the ground state. In fact, shapes connected by conformal transformations have been observed in the microscope.

At finite temperature fluctuations around these shapes of minimal energy are populated according to the usual Boltzmann (Gibbs) factor. Two examples are fluctuations around a mean spherical shape and fluctuations between two energetically equivalent ellipsoids, a prolate and an oblate.

For a review article: U. Seifert, *Advances in Physics* 46, 13-137 (1997).

Topological characterization of porous media for modelling flow and transport

HANS-JÖRG VOGEL

Topology is critical for flow and transport in porous media. This is true both at the pore scale, which may be represented as a binary structure, and at a larger scale defined by continuous macroscopic state variables as phase density, porosity or permeability. At the pore scale a connectivity function is introduced which is defined by the Euler characteristic as a function of the pore diameter. This function is used to generate network models of the porous structure that allow to predict bulk hydraulic properties of the material. At the continuum scale the structure is recorded on a grey scale representing the porosity of the material with a given resolution. Here, topology is quantified by a connectivity function defined by the Euler characteristic as a function of a porosity threshold. Results are presented for the structure of natural soils measured by X-ray tomography. The significance of topology at the continuum scale is demonstrated through numerical simulations. It is found that the effective permeabilities of two heterogeneous random fields having the same autocovariance but different topology differ considerably.

Fitting Boolean Models to Binary Images

RICHARD WILSON

(joint work with Ian Phillips (Queensland))

Many images obtained in materials science, mineral exploration and other areas of engineering and science, consist of polygonal particles of one substance against a background of other substances. The location, shape and size of these particles is often random within certain constraints. For example, the particles may all be convex or they may cluster into groups. Such images can be modelled using random closed sets. A wide class of random set models appropriate for images with these properties is provided by *germ-grain* models. In this talk, we will concentrate on examining the *Boolean* model and methods for fitting

it to data. In particular, we will assume that the grains are convex stable sets and discuss some aspects of parameter estimation. This work is currently in progress, so the talk will focus on some of the background needed, the results so far and work still to be done.

Limit Theory for Random Packing and Deposition

JOSEPH E. YUKICH

Consider sequential packing of unit balls in a large cube, as in the Rényi car-parking model, but in any dimension and with finite input. We prove a law of large numbers and central limit theorem for the number of packed balls in the thermodynamic limit. We prove analogous results for numerous related applied models, including cooperative sequential adsorption, ballistic deposition, and spatial birth-growth models.

The proofs are based on a general law of large numbers and central limit theorem for “stabilizing” functionals of marked point processes of independent uniform points in a large cube, which are of independent interest. “Stabilization” means, loosely, that local modifications have only local effects.

Fractal and aggregate tessellations

SERGEI ZUYEV

Consider a sequence of stationary tessellations $\{\Theta^n\}$, $n = 0, 1, \dots$ of \mathbb{R}^d consisting of cells $\{C^n(x_i^n)\}$ with the nuclei $\{x_i^n\}$. An aggregate cell of level one, $C_0^1(x_i^0)$, is the result of merging the cells of Θ^1 whose nuclei lie in $C^0(x_i^0)$. An aggregate tessellation Θ_0^n consists of the aggregate cells of level n , $C_0^n(x_i^0)$, defined recursively by merging those cells of Θ^n whose nuclei lie in $C^{n-1}(x_i^0)$.

We find an expression for the probability for a point to belong to a typical aggregate cell, and obtain bounds for the rate of its expansion. We give necessary conditions for the limit tessellation to exist as $n \rightarrow \infty$ and provide upper bounds for the Hausdorff dimension of its fractal boundary and for the spherical contact distribution function in the case of Poisson-Voronoi tessellations $\{\Theta^n\}$.

Edited by Gunter Döge

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