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学位（専攻分野）	博士（統計科学）
学 位 記 番 号	総研大甲第992号
学位授与の日付	平成１８年９月２９日
学位授与の要件	複合科学研究科　統計科学専攻 学位規則第６条第１項該当
学 位 論 文 題 目	Bayesian Estimation of Repulsive Interaction Potential Models for Spatial Point Patterns
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論文内容の要旨

A spatial point pattern is a set of locations of points (objects), irregularly distributed within a designated region and presumed to have been generated by some form of stochastic mechanism (Diggle (2003)). Each point is considered as a particle, individual of animals or plants, and so on. During a few decades, the methods of statistical analysis for spatial point patterns have been developed: various diagnostic statistics and graphs have been studied by using the second-order and the nearest-neighbor distance methods (Ripley (1977, 1979a, 2004), Besag (1977), Diggle (1979, 2003)); by clumping indices based on the quadrate methods (David and Moore (1954), Morisita (1954), Lloyd (1967)) or based on the distance methods (Hopkins and Skellam (1954)). Modelling spatial point patterns for which interactions exist between individuals has been studied by some authors (see for example Mat'ern (1960), Ripley (1977), Ogata and Tanemura (1981, 1984)). Spatial point patterns are generally classified into three types: *completely random, clustered* (*aggregated*) and *regular*. If we observe a point pattern where a certain repulsive force is acting between individuals, the pattern is called a regular type. For example, if territorial animals or plants live in a habitat, a certain spacing out among them happens. Besides if birds fly in formation or fish swim in shoals, inhibitions between the individuals realize. In other case, if few or many nanometer- or micrometer-sized dust particles are immersed in a plasma, then the particles with charge form two- or three-dimensional dust Coulomb crystals. In outer space, the crystals can be observed such as the ionosphere or commentary tails, *etc*. In the laboratory, the circular symmetry of the confining potential and the interaction with the mutual repulsion lead to dust Coulomb crystals, which can be observed by the naked eyes through the CCD camera with applying the laser light. Then the behavior of charged dust particles and the structure of the crystals has been investigated (*e.g.* Melzer *et al.* (1994), Nitter (1996), Juan *et al.* (1998), Thomas and Watson (1999), Lai and Lin (1999)).

Many regular point patterns are observed in nature, then we wish to study the stochastic mechanism of the regular patterns. In this thesis, we are particularly interested in the interaction between individuals and it will be interesting to describe this certain spacing out by a repulsive interaction potential. Then we consider these interactions between individuals by repulsive interaction potential models.

We assume that a given regular point pattern is in equilibrium under a certain repulsive interaction potential in a finite two-dimensional region. It is known that such an equilibrium point pattern is statistically represented by the Gibbs distribution. The likelihood of parameters which characterize the interaction potential can be described by the Gibbs distribution for a given equilibrium point pattern. Since the form of the normalizing factor of the Gibbs distribution is a high multiplicity of integral, it is very difficult to obtain the likelihood function in principle. For this reason, Bayesian analysis for these spatial point patterns has been hardly studied. Then, we use the useful approximate log-likelihood (Ogata and Tanemura (1989)), which will be described in Chapter 3.2, and consider our Bayesian estimation of various regular point patterns. Bayesian inference may help us to sensitively estimate parameters of the interaction potentials. The essential characteristic of Bayesian methods is their explicit use of probability for quantifying uncertainty in inferences based on statistical data analysis (Gelman *et al.* (2004)). Because of the development of recent computational methodology, the complex posterior density can be simulated by using MCMC (Markov chain Monte Carlo) methods.

In this thesis, our main purpose is as follows. For a point pattern of repulsive by interacting points in a finite two-dimensional region, we propose a method to obtain the posterior density of the parameters of the parameterized interaction potential functions by using MCMC methods. There, the effective approximate log-likelihood for the models (Ogata and Tanemura (1989)) plays an important role in the Metropolis-Hastings algorithm. Then two types of prior densities corresponding to the parameters of the repulsive interaction potential models are considered. Jumping (proposal) densities with similar type as prior density are applied in Markov chain simulations. Our Bayesian inference is confirmed by applying to various simulated equilibrium point patterns which are generated from MCMC of the Soft-Core models for the cases of large and relatively small number of points. In order to obtain posterior inference for real data sets, we consider the fitting of posterior densities to some parametric functions.

Moreover, MCMC convergence of iterative simulation is also investigated in detail. In the thesis, the approach of single long run is adopted. After a long time iterative simulation have been run in the Metropolis-Hastings algorithm, there are following important problems: when should we begin and finish sampling?, *i.e.* when does the run begin to reach stationary and when should we terminate the run? To solve these problems, we evaluate the burn-in and the stopping time of our single long run based on independent simulated multiple short runs with various starting points (Gelman and Rubin (1992), Cowles and Carlin (1996), Gelman *et al.* (2004)), which will be remarked in Chapte5.3 and 8.2.

The layout of the thesis is as follows. In Chapter 2, a log-likelihood of parameters for equilibrium point pattern is given. In Chapter 3, the repulsive interaction potential models (Soft-Core potential models) with two parameters and their effective approximate log-likelihood are introduced. In Chapter 4, the fundamentals of Bayesian inference for the Soft-Core models are described. In Chapter 5, the Metropolis-Hastings algorithm for Bayesian inference, its jumping rule and assessment of the convergence (the burn-in and the stopping time) from iterative simulation are stated. In Chapter 6, firstly, our Bayesian estimation procedure is applied to various simulated equilibrium point patterns which are generated by MCMC methods of the Soft-Core models for the cases of large and relatively small number of points. Then MCMC convergence is evaluated and the comparison of marginal posterior densities of parameters under two types of the prior densities is also shown. In Chapter 7, four real data sets are illustrated. Then as a preliminary analysis, we classify the type of distribution of each point pattern. In Chapter 8, the results of our Bayesian estimation of the Soft-Core models for these real data sets are shown. There, the assessment of MCMC convergence is investigated in detail. In order to obtain posterior inference from iterative simulation, parametric fitting of the generalized gamma distribution to marginal posterior densities is considered. To examine the validity of our results, the L-statistics for observed data is compared graphically with the envelopes of simulated point patterns for the posterior mode of model parameters. We then make reference to the literature of Okabe and Tanemura (2006). Finally, in Chapter 9, some concluding remarks are given.

論文の審査結果の要旨

提出された学位申請論文 9 章 105 頁からなり、英語で執筆されている。本研究の目的は、平面上に与えられた点配置データから、点間に働くと想定される反発型相互作用ポテンシャル関数の形状を決める 2 つのパラメータの値を MCMC 法を用いてベイズ推定することである。所与の点配置データに Gibbs 分布を仮定して相互作用ポテンシャルの形状を推定するための方法は Ogata- Tanemura (OT) などによって早くから提案されているが、パラメータに事前分布を設定してベイズ推定を行う点に新規性が主張されている。本論文の第 2,3 章は本研究で利用する OT の提案した近似尤度の説明を中心に概説している。第 4 章ではベイズ的手法の枠組みの概説と本研究で用いられる 2 種の事前分布（一様分布、切断正規分布）の導入がなされている。第 5 章では Metropolis-Hastings による MCMC アルゴリズムの説明がなされ、その際、このベイズ的手法では近似尤度における正規化定数の利用が本質的であることが述べられている。また MCMC 標本系列の収束診断のために Gelman-Rubin 判定量が導入されている。第 6 章ではシミュレーション・データに対して、反発型（soft-core 型）ポテンシャルのパラメータのベイズ推定法をいくつかのパラメータ値の組み合わせに対して検証し、本研究で提出しているベイズ的手法が真のパラメータ値に対応する事後分布の導出に有効であることを示している。第 7 章は手法を適用する実データの説明と予備的解析の記述であり、第 8 章ではそれらのデータに対する soft-core 型ポテンシャルのベイズ推定の結果が述べられている。ここでは結果に対する感度解析の一環として、事後分布からの標本値に対して生成されたシミュレーション・データと元の実データとの間で K-関数（L-関数）による診断的比較が行われ、両者の間の一致が概ねすべての実データに対して得られている。その際、MCMC 標本系列から得られた事後（頻度）分布に一般化ガンマ分布を当てはめた簡略化表現が利用されている。

本論文の第 6, 8 章において OT の soft-core 型ポテンシャルに関する近似尤度を用いた MCMC によるベイズ推定法をシミュレーション・データおよび実データに対して実証的に確認したことは高く評価できる。また、Gelman-Rubin 判定量を用いるなど、収束の判定にも十分に配慮されており、MCMC 法の実用的観点から評価できる。また、データ数が少ないシロガシラハイイロカモメ(N=110)のポテンシャルのベキに関するパラメータを除けば、事前分布の形がパラメータの事後分布に影響しない結果を得ており、提案する手法に頑健さがあり、他のデータにも適用可能であると推測できる。このように、MCMC 法を用いて点配置データを解析する手法を発展させた点に，統計科学への貢献が認められる。

なお、本研究の主内容に関係した申請者を筆頭著者とする英文論文が日本統計学会英文誌に掲載予定である。

以上から、博士論文審査委員会は、申請者の学位請求論文が学位に十分値する水準にあると全員一致で判定した。