氏名
岡部 正浩

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学位論文題目
Bayesian Estimation of Repulsive Interaction Potential Models for Spatial Point Patterns

論文審査委員
主査教授
田村 義保
教授
種村 正美
教授
尾形 良彦
教授
伊藤 栄明
助教授
伊庭 幸人
教授
間瀬 茂 (東京工業大学)
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 quadrat 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 Matern (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 ionsphere 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. The 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 Chapters 5.3 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、点間で働くと考え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、パラメータの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章では手法を適用する実データの説明と推定解析の実例であり、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用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コモド（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連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。