Application of Parameter Estimation for Diffusions and Mixture Models

The first part of this thesis proposes a method to determine the preferred number of structures, their proportions and the corresponding geometrical shapes of an m-membered ring molecule. This is obtained by formulating a statistical model for the data and constructing an algorithm which samples from a posterior distribution. The sampling algorithm is constructed from a Markov chain which allows the dimension of each sample to vary, this is obtained by utilizing the Reversible jumps methodology proposed by Peter Green. Each sample is constructed such that the corresponding structures are physically realizable; this is obtained by utilizing the geometry of the structures. Determining the shapes, number of structures and proportions for an m-membered ring molecule is of interest, since these quantities determine the chemical properties. The second part of this thesis deals with parameter estimation for diffusions. The first idea is in an optimal way to incorporate prior information in the estimation equation $G(X_{t1}; \ldots; X_{tn}) = 0$, used to nd an estimator of the unknown parameter $\theta$. The general idea is to introduce an new optimality criterion which optimizes the correlation with the posterior score function. From an application point of view this methodology is easy to apply, since the optimal estimating function $G(X_{t1}; \ldots; X_{tn})$ is equal to the classical optimal estimating function, plus a correction term which takes into account the prior information. The methodology is particularly useful in situations where prior information is available and only few observations are present. The resulting estimators in some sense have better properties than the classical estimators. The second idea is to formulate Michael Sørensen's method "prediction based estimating function" for measurement error models. This is obtained by constructing an estimating function through projections of some chosen function of $Y_{t+1}$ onto functions of previous observations $Y_{t}; \ldots; Y_{10}$. The process of interest $X_{t+1}$ is partially observed through a measurement equation $Y_{t+1} = h(X_{t+1}) + \text{noise}$, where $h(\cdot)$ is restricted to be a polynomial. Through a simulation study we compare for the CIR process the obtained estimator with an estimator derived from utilizing the extended Kalman filter. The simulation study shows that the two estimation methods perform equally well.
Bayesian methods for the conformational classification of eight-membered rings

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Solid state conformational classification of eight-membered rings
A statistical classification of the solid state conformation in the title complexes using data retrieved from the Cambridge Structural Database (CSD) has been made. Phosphate and phosphinate complexes show a chair conformation preferably. In phosphonate complexes, the most frequent conformations are found to be boat–chair, chair and boat–boat; in all the boat–chair cases, the phosphorus atoms appear connected by a bridging carbon atom.

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Supervisor:

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