AN IMPROVED TWO-STEP METHOD IN STOCHASTIC DIFFERENTIAL EQUATION'S STRUCTURAL PARAMETER ESTIMATION

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To my parents, mother in law, husband and children.

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ABSTRACT

Non-parametric modelling is a method which relies heavily on data and motivated by the smoothness properties in estimating a function which involves spline and non-spline approaches. Spline approach consists of regression spline and smoothing spline. Regression spline characterised by the truncated power series basis with Bayesian approach is considered in the first step of a two-step method for estimating the structural parameters for stochastic differential equation (SDE). Previous methodology revealed the selection of knot and order of spline can be done heuristically based on a scatter plot. To overcome the subjective and tedious process of selecting the optimal knot and order of spline, an algorithm is proposed. A single optimal knot is selected out of all the points with exception of the first and the last data and the least value of Generalised Cross Validation is calculated for each order of spline. The spline model is later utilised in the second step to estimate the stochastic model parameters. In the second step, a non-parametric criterion is proposed for estimating the diffusion parameter of SDE. Linear and non-linear SDE consisting of Geometric Brownian Motion (GBM) for the former and logistic together with Lotka Volterra (LV) model for the later are tested using the two-step method for both simulated and real data. The results show high percentage of accuracy with 99.90% and 96.12% are obtained for GBM and LV model respectively for diffusion parameters of simulated data. This verifies the viability of the two-step method in the estimation of diffusion parameters of SDE with an improvement of a single knot selection.

ABSTRAK

Permodelan tak berparameter ialah satu kaedah yang sangat bergantung kepada data dan bermotivasikan kelicinan dalam menganggar fungsi yang melibatkan pendekatan splin dan bukan splin. Pendekatan splin terdiri daripada splin regresi dan splin pelicinan. Regresi splin berunsurkan siri asas kuasa terpangkas dengan kaedah Bayesian digunakan dalam langkah pertama untuk kaedah dua-langkah bagi menganggar parameter struktur persamaan pembeza stokastik (SDE). Metodologi terdahulu menunjukkan bahawa pemilihan simpulan dan tertib splin boleh dilakukan secara heuristik berdasarkan plot serakan. Untuk mengatasi proses pemilihan bilangan simpulan dan tertib splin yang subjektif dan memakan masa, satu prosedur penyelesaian dikemukakan. Simpulan tunggal terbaik dengan nilai pengesahan silang teritlak minimum dipilih dari semua titik kecuali data pertama dan terakhir. Model splin yang terhasil kemudiannya digunakan dalam langkah kedua untuk menganggar parameter model stokastik. Dalam langkah kedua satu kriteria tak berparameter telah dicadang untuk menganggar parameter pembauran model persamaan pembeza stokastik. Persamaan pembeza stokastik linear dan tak linear terdiri daripada model Gerakan Geometri Brown (GBM) dan model logistik beserta model Lotka-Volterra diuji (LV) menggunakan kaedah dua-langkah bagi data cerapan dan data simulasi. Hasil kajian menunjukkan peratus ketepatan yang tinggi iaitu 99.90% dan 96.12% diperoleh untuk model GBM dan LV masing-masing bagi parameter pembauran dengan menggunakan data simulasi. Ini mengesahkan kebolehjayaan kaedah dua-langkah menggunakan kriteria tak berparameter yang dicadang dalam menganggar parameter pembauran model persamaan pembeza stokastik dengan menambahbaik kaedah pemilihan simpulan tunggal.

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LIST OF SYMBOLS/ABBREVIATIONS/NOTATIONS

$\mathrm{E}(X)$	–	Expected value of X
f'	–	First derivative
f''	–	Second derivative
ε	–	Random Error
g	–	Gram
h	–	Hour
L	–	Liter
MSE	–	Mean Square Error
ODE	–	Ordinary Differential Equation
t	–	Data points/time
SDE	–	Stochastic Differential Equation
$\mathrm{Var}(X)$	–	Variance of X
$W(t)$	–	Wiener process
x	–	Concentration of cell mass (g/L)
x_{max}	–	Maximum cell concentration
YE1	–	Control medium
YE2	–	Medium of Yeast and $(NH_4)_2SO_4$
YE3	–	Medium of Yeast and $NH_4H_2PO_4$
YE4	–	Medium of Yeast and NH_4Cl
YE5	–	Medium of Yeast and NH_4NO_3
$\mathbb{R}$	–	Real number
Δ	–	Step size
μ_{max}	–	Maximum specific growth rate
$\emptyset$	–	Empty set
Ω	–	Sample space
ϕ	–	Diffusion coefficient

$\hat{\phi}$	–	Estimated diffusion coefficient
$\phi*$	–	True diffusion coefficient
$\subseteq$	–	Subset
$\in$	–	Element
θ	–	Average drift coefficient
θ^*	–	True average drift coefficient
$\hat{\theta}$	–	Estimated drift coefficient
x_0	–	Initial value of dependent variable
$f(t)$	–	Regression function
ζ	–	Knot
α,δ	–	Regression spline coefficient
ε	–	Random error
B_i^k	–	*K*th order of B-splines
υ	–	B-spline coeffient
ϱ	–	Coefficient of natural cubic spline
ν, τ	–	Smoothing spline parameters
Z, z	–	Standard normal variable
Σ	–	Summation
$\|x\|$	–	Modulus of x
$\|\|x\|\|$	–	Norm of x
x^*	–	True solution of ODE
$\dot{x}^*$	–	Derivative of true solution of ODE
$\widehat{x}_n$	–	Consistent estimator of true solution of ODE
$\widehat{\dot{x}}_n$	–	Consistent estimator of derivative of true solution of ODE

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CHAPTER 1

INTRODUCTION

1.1 Introduction

Many physical phenomena can be better presented and understood via mathematical modeling. Wide range of literatures on mathematical modeling of physical system may be found with deterministic modeling particularly by deterministic differential equation whereby the element of noise is not considered. Deterministic differential equation describes a model of physical system and is solved to explain how a system changes or develops, when change occurs and the effect of the starting point to the initial solution and so forth. It represents idealised situations and can be improved by introducing stochastic element since in reality many phenomena in nature are affected by stochastic noise and Stochastic Differential Equations (SDE) may be required. Some of the fields which apply SDE are in finance (Aguilera *et al.*, 1999), (Henderson, 2005), (Cifarelli and Tagilani, 2002), in population dynamics (Bahar, 2005), (Kamina *et al.*, 2000), (McKane and Newman, 2004), in engineering (Ló *et al.*, 2008), (Li *et al.*, 2012) (Sogutlu and Koc, 2007) and in biometry (Garcia, 1983), (Goulding, 1994), (Preisler *et al.*, 2004).

The perturbation or random fluctuation included in the function and the stochastic modeling can be considered from the corresponding Itô or Stratonovich differential equations or from the associated Kolmogorov (Fokker-Planck and backward) differential equations (Gutiérrez *et al.*, 2008). All the above differential equations represent the extrinsic stochasticity wherein the stochasticity is introduced by incorporating multiplicative or additive stochastic terms into the differential equation. Extrinsic stochasticity is due to random variation of one or more environmental or external factors such as temperature of concentration of reactant species, whereas intrinsic stochasticity is inherent to the system, which arises due to the relatively small number of reactant molecules. Intrinsic stochasticity can be described by a chemical master equation (Gillespie, 1977) as in APPENDIX I. Only external random fluctuations or external stochasticity will be considered in this work. The general form of the SDE consist of deterministic or average drift term and a diffusion term. The element of noise is contained alongside with the diffusion term and represented by Brownian motion.

1.2 Research Background

Classical parametric estimator for stochastic differential equation includes Maximum Likelihood Estimation (MLE), methods of moment, Least Squares Estimation (LSE) and Kalman filtering. The drawback of the first method is the requirement of the transition density function which is sometimes unavailable in some SDE functions. In MLE, the numerical approximation of transition density function is computed with numerical approximation. Three methods of numerical approximation include solving numerically the Kolmogorov partial differential equations satisfied by the transition density (Lo, 1988) or deriving a closed-form Hermite expansion to the transition density (Egorov *et al.*, 2003) and lastly simulating R times of the process using Monte-Carlo to integrate the transition density (Durham and Gallant, 2002), (Pedersen, 1995), (Hurn *et al.*, 2003). The third approach is also known as Simulated Maximum Likelihood (SML). Picchini noted that the first and the last approach are computationally intense and poorly accurate while the second method is accurate and fast, applicable over a wide range of SDE models (Picchini, 2006).

However, the main drawback of the second method is computing the Hermite expansion of the transition density. It could be a very difficult task if the SDE is multivariate and non-linear and it is only available for small number of models. Instead of considering to estimate the parameters of SDE with likelihood approach, we opt to take fully non-likelihood approach by applying the two-step method used in estimating parameters of SDE with non-parametric approach. The application of non-parametric approach in SDE in previous studies includes the estimation of trends for stochastic differential equations with kernel type estimator or kernel function technique (Mishra and Rao, 2011), (Federico and Phillips, 2003), (Nicolau, 2008). Nevertheless, in Two-step method the purpose is to estimate SDE parameters with spline technique with Bayesian approach which is considered quite distinct from previous works.

1.3 Problem Statement

The motivation of this work is to estimate the structural parameters of SDE by implementing some non-likelihood approach. This is due to the difficulty in the existing technique which involves the estimation of the likelihood density functions. Classical methods such as Maximum Likelihood Estimation (MLE) require complex computational procedures. In this study, a non-parametric approach with regression spline is considered in the first step since it is considered easier and more flexible than smoothing spline. Truncated power series basis is utilised in favour to B-spline basis. This would be an advantage, since if B-spline is used instead when choosing fewer knots, it will show a non-local behaviour pattern. The estimation of regression spline parameters will be done by implementing the Bayesian approach with Winbugs software in this research, since it provides a more exact inference and faster simulation time.

Classical methods such as MLE is considered difficult in ODE parameter estimation because of the implicit dependence of the independent variable x on the parameter, which prohibits proper maximization of the likelihood function. Derivative-based methods like Newton-Raphson are not easy to handle and evaluation of the likelihood necessitates the integration of the ODE, which becomes a burden when a huge parameter space needs to be explored. The same problem would persist relating to MLE approach in SDE opting us to consider non-likelihood approach in the Two-step procedure. In the second step the estimation of the parameters of the drift term will be done utilizing a criterion from existing literature. To estimate the parameter of the diffusion term a new non-parametric criterion will be proposed. This approach is expected to be simpler since it does not involve the estimation of the likelihood density function and may be an alternative to classical likelihood approach, thus, avoiding the computational difficulties encountered by such method.

1.4 Research Objectives

The objectives of this study are:

1. To propose a Two-step method in the parameter estimation of SDE.
2. To assess empirically the methods of estimating SDE parameters using simulated and real data of Geometric Brownian Motion for linear and Logistic models and Lotka-Volterra for non-linear models with the above-mentioned method.
3. To compare the Two-step method with MLE and LSE.

1.5 Research Scope

The incorporation of stochasticity is only restricted to extrinsic stochasticity, where only external random fluctuations from Itô stochastic differential equation are taken into consideration. Only regression spline with truncated power series basis is considered with a single knot location. Besides, only one dimensional stochastic models are considered in the empirical assessment of the proposed Two-step method including Geometric Brownian Motion with Opening Share Prices set of data for real application, and Power Law Logistic models in modeling the cell growth of the fermentation process. The stochastic modeling is only imposed on the direct batch fermentation of acetone-butanol ethanol (ABE).

1.6 Siginificance of Research

In this research, the parameters estimation of SDE is presented in a novel way with a total non-likelihood approach by deriving the non-parametric criterion for the estimation of diffusion term parameter for general case of SDE. This serves as an alternative to the existing methods of estimating the parameters of SDE. A non-parametric criterion introduced by Varah (1982) is utilised to estimate the average drift parameter of SDE and a proposed criterion to estimate the diffusion parameters. This approach exclude the approximation of the probability density function in classical methods such as MLE. It hopes to avoid difficulty and complexity of the computational aspect of such approach.

In this work proving of consistency of the proposed non-parametric criterion of diffusion parameter estimate is also provided. The proof has shown that the non-parametric estimator is indeed consistent and deemed to be a good estimator. Another contribution includes the derivation of an information criterion which acts as a stopping criterion which stops the procedure of finding the best diffusion parameters estimate when the required optimality objective is achieved.

The Stochastic Non Parametric Criterion coined as SNPIC is derived based on the non-parametric criterion proposed. Results show the utilization of SNPIC as stopping criterion produced highly accurate estimate of diffusion parameter from simulated data and is depicted by high percentage of accuracy when compared to the initially fixed parameters.

To simplify the process of single knot selection in the first step, an algorithm is introduced by iteratively calculating the values of GCV with each data except the first and the last one acting as single knot. GCV is a numerical measure where the least value of GCV will indicate the best knot selection. This approach is a novel application to Bayesian regression spline with Winbugs software. Bayesian estimation in regression spline is preferred since it provides a more exact inference and faster simulation time (Crainiceanu *et al.*, 2005).

In the area of biotechnology, especially in the kinetic modeling of fermentation, majority of the literatures found had employed deterministic modeling. In the case of ABE fermentation, the application of stochastic modeling via non-parametric modeling is unavailable. This research is done to fill the gap in the literatures and give new highlight to a more realistic and meaningful aspect of modeling physical or natural phenomena primarily in ABE fermentation process and other biological modeling.

1.7 Thesis Organisation

Organisation of the thesis is as follows. Chapter 1 discusses some issues regarding parameter estimation of SDE in general followed by the problem statement, research objectives, research scope, significance of research and thesis organisation. Chapter 2 highlights literature reviews of SDE parameter estimation followed by non-parametric modeling and methods of parameter estimation in non-parametric modeling. Lastly, the Two-step method in ODE and SDE is described along with the literature reviews. Chapter 3 explains the details of the methods in parameter estimation of SDE such as simultaneous estimation in least squares method and maximum likelihood estimation. It also discusses on the Two-step Method in ODE and SDE with the derivation of the non-parametric criterion for the estimation of the diffusion parameters shown together with the proving of its consistency. The verification and application of the Two-step method are described in Chapter 4 and 5 with simulated and observed data for linear SDE and non-linear SDE. For linear SDE, the result is compared with method of MLE and for non-linear SDE the result is compared with simultaneous estimation in least squares method. Chapter 6 discusses the conclusions and suggestion for further work.

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