Stochastic and numerical modelling of anomalous diffusion signals

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SUMMARY

The purpose of this dissertation is to propose an apparatus to stochastically and numerically model the anomalous diffusion signals. We use the term "anomalous diffusion process" in the sense that a stochastic process $X(t)$ has the mean-squared displacement described by

$$\mathbb{E}\left(X(t) - X(0)\right)^2 \sim t^a \quad \text{for some } a > 0.$$

Deviations of the exponent a from 1 lead to the notion of anomalous diffusion: $a \in (0, 1)$ corresponds to subdiffusion, $a > 1$ to superdiffusion, whereas $a = 1$ stands for the standard diffusion. Our main goal is to propose strict methodology of identification and validation of the analysed anomalous diffusion models. We consider various anomalous diffusion models, such as: fractional Brownian motion, fractional Gaussian nosie, fractional stable motion and autoregressive fractionally integrated moving average (ARFIMA) processes. The main focus of this dissertation is the, so called, toy model, i.e. sum of fractional Brownian motion and independent white Gaussian noise, which will serve as a basic model for fractional anomalous diffusion with measurement noise.

In Chapter 1 we introduce the concept of anomalous diffusion. We present the models which are used thereafter and some of their characteristics.

In Chapter 2 we extend the, known in the literature, weighted least squares estimator of the diffusion coefficient to the toy model to obtain estimators of the diffusion coefficient and the magnitude of the measurement noise. Our main result of the second chapter is Theorem 2.1 presenting the formulas for the toy model parameter estimators, and Theorem 2.5 stating that those estimators are unbiased.

In Chapter 3 we analyse the FIMA$(d, 1)$ model and its connection to the toy model. We justify the usage of the toy model which takes the experiment noise into consideration. The main results of the third chapter are two

algorithms, namely Algorithm 1 and Algorithm 2. Algorithm 1 can be used to generate the calibration surface for the FIMA model, whereas Algorithm 2 can be used to estimate the anomalous exponent α and magnitude of the measurement noise σ using the calibration surfaces. We also present an example, which shows the advantage of using calibration surfaces method over the standard mean-squared displacement (MSD) method.

In Chapter 4 we consider the topic of ergodicity of a stochastic process. We present two approaches – the first is analytic and can be applied to Gaussian processes, while the second is numerical and can be used to general infinitely divisible processes. The main results of Chapter 4 are Theorems 4.7 and 4.8 describing the distribution of the statistics related to the notion of ergodicity of Gaussian processes, Algorithm 4 applying the results of Theorem 4.8 to calculation of the quantiles of the sum of autocovariance function, and also Algorithm 3, which can be used to numerically calculate the so-called ergodic surface from which we can obtain the quantiles of the dynamical functional. Also, in this chapter we use Monte Carlo simulations to compare the analytical formula for the characteristic function for the statistics described in Theorems 4.7 and 4.8 with the corresponding empirical characteristic function. We also apply both theorems to the toy model.

Chapter 5 has a more applicable character. We describe a step-by-step algorithm on how to analyse a real signal by using previously introduced methods. Finally, we apply it to biological data.

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