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Spatial Effects in Stochastic Microscopic Models - Case Study and Analysis

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Abstract: In this paper we are going to present techniques to investigate the theoretical background of so called microscopic models (i.e. models consisting of a large number of individual but yet cooperating actors). We will lay special emphasis on the analysis of so called aggregated numbers, hereby speaking of usually scalar, summarising variables, dependent on all actors simultaneously, which are typically some kind of sums or statistics. We are going to analyse the behaviour of those quantities in case of a very large number, respectively in the limit case, an infinite number of individual actors. We will especially focus on the influence of spatial relationships between the actors on the aggregated number. Stochastic methods are going to play the key role in this theory. Furthermore we will apply the results of the theoretical research on three different microscopic models, each of them chosen to particularly point onto an important observation. The first model, a simplified epidemics model, is going validate the theory and demonstrates how to use it. The second model, based on famous *Game of Life* by John H. Conway, will reveal the limits of the method and finally, the third model, an extension of the second one, will show the benefits and applicability of the analytically derived theory.

Keywords: Microscopic Modelling, Agent-Based Modelling, Diffusion Approximation, Mean-field Approximation, Aggregation, Markov-Process

1. INTRODUCTION

The term *microscopic*, often used by modelling experts to communicated a basic idea about a certain model is, almost independent of the scientific research field, usually associated with a *lot* of individual actors or particles (inter)acting in a certain environment. Any further interpretation is difficult and might be misleading as there is no global definition of the term *microscopic* respectively *microscopic model* all scientific fields agree with. E.g. physicists might receive motivation developing microscopic models by needs of spatial discretisation of a liquid via simple particles (Chen and Doolen (1998)), whereas computer engineers might be motivated by simulating highly complex behaving human (Bruckner et al. (2012)).

In context of our work we will use the term *microscopic* model for dynamic (hereby used to indicate temporal dependent) models, consisting of a high number of similar sub-models, which will furthermore be denoted as *actors*. Hereby the idea of increasing the number of actors has to be possible and meaningful in the specific context. By the term we want to cover big classes of models like e.g. agent-based models, cellular automata or microsimulation models. As a microscopic model does not necessarily contain a spatial structure we will focus on those kind of models. Nevertheless the presented technique can also be applied on models without spatial relationships.

In this paper we will not discuss different motivations and applications of microscopic models, but are going to present a technique to investigate the theoretical background of microscopic models. We will lay special emphasis on the analysis of so called aggregated numbers, typically some kind of sums or statistics. We are going to analyse the behaviour of those quantities in case of a very large number, respectively in the limit case, an infinite number of individual actors. We will especially focus on the influence of spatial relationships between the actors on the aggregated number. Furthermore we will apply the results of the theoretical research on three different microscopic models, each of them chosen to particularly point onto an important observation.

2. ANALYTICAL METHODS

As a part of the complex-systems-theory (see Wolfram (1988)) the analysis of microscopic models, especially those in which actors depend on each other during runtime, is generally motivated by possible emergence of unexpected and sometimes even chaotic effects. Hereby unexpected describes the necessity to simulate the whole model in order to make any prognosis for the simulation-output at all. This is different e.g. for differential equation models for which a steady state analysis can be performed. It is not surprising that it is hardly possible to predict the behaviour of a single sample actor as it is dependent on the behaviour of all or at least some other individuals

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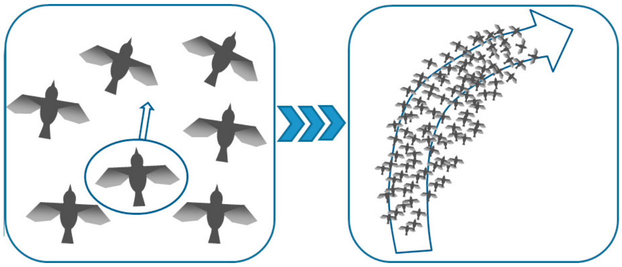

Fig. 1. Unexpected emergent behaviour of the mass on the example of a bird flock. Simple individual rules lead to complex unpredictable behaviour of the flock.

too. However it is surprising that it is also very difficult to predict the behaviour of the whole crowd respectively so called aggregated numbers of the model (see Figure 1). This effect can be seen as a special kind of swarm-intelligence.

2.1 Aggregated Numbers

Aggregated numbers in microscopic models are summaries of the state of all individual actors and are used to describe the overall state of the model. As already mentioned they are sometimes simple statistics of the actors like mean or variance of the individual states. We furthermore define that a function a is called *aggregation function* of a microscopic model consisting of m_i, $i = 1 \dots N$ actors with corresponding states $\vec{s}_i \in \Gamma$ if it fulfils the following properties:

(1) $a : \prod_{i=1}^{N} \Gamma \to K \subseteq \mathbb{R}^d,\ (\vec{s_1}, \dots, \vec{s_N}) \mapsto a(\vec{s_1}, \dots, \vec{s_N})$
(2) K is independent of N and compact
(3) $a(p(\vec{s_1}, \dots, \vec{s_1})) = a(\vec{s_1}, \dots, \vec{s_1})$ for all permutations p

Property (2) guarantees that the function-output is qualitatively independent of the number of actors. Especially $a(\vec{s_1}, \dots, \vec{s_N})$ remains finite if $N \to \infty$. Property (3) provides that all actors are treated the same way and no index is preferred. Outputs of this function are finally called aggregated numbers. As the states $s_i(t)$ are time-dependent so is usually $a(t)$. Of all aggregation functions surely the empiric mean and the empiric variance are the best known. Here we want to introduce a slight adaptation of the empiric mean which will furthermore pose the basis for analytic research. The aggregation function

$$o_k(\vec{s_1}, \dots, \vec{s_N}) := \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}_k(s_i), \tag{1}$$

with the indicator function $\mathbb{I}_k(x) = \delta_{k,x}$, will be called *counting function* of the state k as is counts the fraction of all actors currently sharing this state. The output of this function is furthermore called *counting variable* or *counting vector* and can be calculated for all possible states k of the actors. If the number of possible states is discrete, the counting variables fulfil $\sum_k o_k = 1$.
To understand the following chapters it is crucial to notice that we hereby projected a system consisting of N actors, each having one of d different states at a time, onto a system consisting of d different state variables, each taking values between zero and one (see Figure 2).

Target of the following sub-section is the prediction of the temporal development of the counting function for

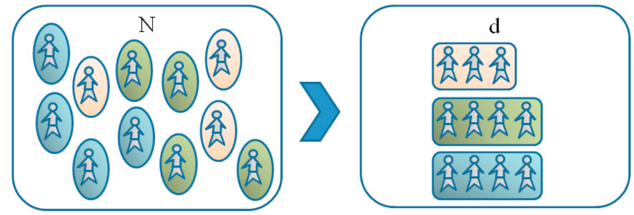

Fig. 2. Graphical interpretation of the principle of the counting function defined in (1).

simplified stochastic microscopic models without directly performing the simulation. As the model is meant to be stochastic also the counting function is a stochastic variable. Hence we will derive formulas for mean and variance of the function.

2.2 Diffusion Approximation

Diffusion approximation of Van Kampen (see Kampen (2007) and Kampen, N. G. van (1982)) respectively at least its results are, by knowledge of the author, still core of all theorems developed to perform aggregated analysis of microscopic models - so called mean-field theorems (some examples: Boudec et al. (2007), Benoit et al. (2006)). Although the same theorems can also be derived by other approaches (like e.g. Itô-calculus) too, we will present the diffusion-approximation method, because knowledge about extended stochastic calculus is not required in order to understand it. Basically the idea was developed to investigate probability-densities of quantum mechanical particles and was reworked and extended several times to enlarge its field of application.

Roots of this method lie within Markov-Theory and, to be more precise, within the Kolmogorow Equation (see Kolmogorov, A (1931)) respectively the discrete part of its differential form, the Master Equation: Given a regular, time continuous and homogeneous Markov process $X(t)$ which only takes discrete values in Ω the following equation holds for its probability function:

$$\frac{\partial P(x,t)}{\partial t} = \sum_{y \in \Omega} P(y,t)\omega_{x,y} - P(x,t)\omega_{y,x}. \tag{2}$$

Hereby $\omega_{x,y}$ are called transition-rates of the Markov process and can be seen as time-derivatives of transition-probabilities. For the derivation of this equation we refer to Gardiner (2009). As discrete, finite state-spaces Γ (compare with the definition of aggregated numbers) is most applicable for the desired test cases we furthermore only consider these, which are furthermore denoted with $\{1, \dots, d\}$.

The main idea of diffusion-approximation respectively mean-field approximation, is to use this equation to express the temporary behaviour of the counting-function as defined in (1). This approach only works correctly if the counting-function itself is a Markov-process. To analyse under which circumstances this feature is given was key objective of this work. The most valuable observation hereby is that the actors itself do *not* necessarily need to be Markov-processes in order to inherit the Markov-property to the counting variables. It is sufficient that the transition probabilities of the individual actors can be written as