Günter Haag

Modelling with the Master Equation

Solution Methods and Applications in Social and Natural Sciences

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Günter Haag
University of Stuttgart
Institute of Theoretical Physics II
Germany

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This book is dedicated to Eva, Manuel and Stephan and all the beautiful outcomes based on chaotic decisions.

Foreword

All of us have to make decisions on our actions, based on our expectations of the future.

This holds true for individuals as well as for institutions such as companies, city councils, state governments, and international agencies. But, as we all know, we live in an ever increasingly complex world with all its uncertainties. Can we find any guidelines how to plan and act? May be even enviously, we look at physics with its high predictive power and technical realizations which allow us to send a rocket to distant planets with high precision. Thus, it is certainly tempting to transfer insights gained in physics to the treatment of social, socio-economic or economic processes. The great predictive power of physics is due to its use of mathematics. In my view, mathematics and its way to think will become more and more important also in areas I just have mentioned.

An important step in transferring concepts from physics to sociology has been done in 1972 by my late friend and colleague Wolfgang Weidlich who could draw a close analogy between the formation of public opinion and order–disorder transitions in magnetism. The mathematical vehicle he used is the master equation that I will discuss below. The author of this book, Günter Haag, was one of Weidlich's prominent students and co-workers. Weidlich and Haag published a monograph on *"Concepts and models of a quantitative sociology: The dynamics of interacting populations"* (1983). As I know from Weidlich, Haag contributed considerably because of both his mathematical skills and his openness for practical applications. This has led, in particular, to the Weidlich–Haag model and to important further contributions e.g. to decision theory and regional planning by very concrete studies, which are also part of this book. But why use the master equation? It provides us with an excellent means to deal with uncertainties. In fact, it allows us to calculate probabilities of future states and thus to study various scenarios of developments. These developments result from purely deterministic relationships—so to speak, stringent laws, and chance events, on which we can make only guesses. The master equation combines these effects. In his book, Haag introduces the basic concepts of probability theory in an easy to understand way, derives the master equations and presents numerous explicit examples of its application in physics, chemistry and especially socio-economics. This book is an important contribution to Synergetics that deals quite generally with the self-organized formation of structures in Nature and Society. Haag's book addresses many problems of great public interest, such as migration and regional planning. I am sure that it will become an important reading for students, professors and practitioners.

Stuttgart
March 2017

Hermann Haken

Preface

Since the last decades, the modelling potential of the Master equation has been widely ignored, especially in the social sciences. Possibly, because the mathematics looks so complicated and a general introduction to the framework of the Master equation and its application was not available. Of course, one has to learn about the solution formalisms and the theory of the Master equation to apply the framework. The best way to do this is often to consider examples and applications of the Master equation in different fields and to learn to apply by doing.

The Master equation provides a general framework for model building in different disciplines like physics, chemistry and biology as examples in the natural sciences and economy, sociology, psychology and geography in the social sciences.

During the last decades, a rather big set of mathematical solution methods for the Master equation have been developed. It depends on the system under consideration which solution method seems to be most appropriate to apply. Therefore, it is one aim of this book not only to present different mathematical solution methods but also to show their potential in case of practical examples.

The book is based on courses of mine in the field of interdisciplinary research held at the University of Stuttgart during the last two decades. And, in fact, some examples of the book are related to those lectures and courses. But some applications and research issues are based on consultancy work of STASA (Steinbeis Applied Systems Analysis GmbH) which I founded in 1995.

To make the book easier to read, it is subdivided into three Parts. Part I comprises Chaps. 1–4 and is dealing with some statistical fundamentals, the derivation of the Master equation, the Fokker–Planck equation and other relevant statistical issues. In addition, solution methods of the Master equation including some rather new solution tools for a group of special problems are presented. Part I is rather technical and can be used as a toolbox.

However, benchmarking of different solution methods is important to learn about the advantages of the Master equation framework compared with other modelling approaches.

Therefore, in Part II and Part III of the book, we do not only apply the Master equation framework to different case studies but also compare it with other solution methods. A set of examples out of the field of physics, chemistry, population dynamics, dynamic decision theory, opinion formation and urban and regional dynamics are treated. However, the main focus of the examples is related to the social sciences. The examples underline the interdisciplinary modelling potential of the Master equation approach.

Of course, it is not necessary to follow in Part II and Part III one chapter after the other. Each chapter can be understood independently of the others. But sometimes it is helpful to compare applications out of different fields, Especially, since different methods of solution are applied and compared.

Since the book is written for graduate students, researchers and professionals, it was my aim to perform all mathematical steps which are relevant to come step by step to the final solution. Furthermore, it was my intention to introduce the reader by additional information to the different fields of application. The examples are selected to explain how the Master equation framework works, but also to introduce into different important interdisciplinary research topics of our scientific community.

The target audience therefore consists of interdisciplinary interested scientists, namely economists, physicists, biologists, geographers, sociologists, computer scientists, mathematicians and psychologists who are interested in modelling, simulations and mathematical methods and real-world applications.

Friendly relations with a number of colleagues from many universities all over the world have influenced the different applications and, therefore, the structure of the book.

A Nato Advanced Study Institute held in July 1982 in San Miniato, Italy, on evolving geographical structures focused my interest on interdisciplinary research of socio-economic space–time processes and patterns as well as real-world planning problems. Many international cooperation and resulting research projects were mainly initiated and supported by conferences and workshops organized and financed by *Deutsche Physikalische Gesellschaft* (DPG), the *International Institute for Applied Systems Analysis* (IIASA), the *Istituto Ricerche Economico-Sociali Del Piemonte* (IRES), the *Institut National D'Etudes Démographiques* (INED) and the *Centre for Regional Science Research Umea* (CERUM) to mention a few. It was not self-evident to find such a friendly acceptance and willingness to cooperate among economists, geographers, sociologists and regional and transport scientists with me as a physicist. This shows, however, that the field of interdisciplinary research is open for new ideas. I wish to thank all of them.

My special thanks go to my friend and mentor Wolfgang Weidlich, who unfortunately passed away far too early. His encouragement and many intensive and fruitful discussions and common work that have taken place over many years made the book possible.

Last but not least, special thanks go to the Springer-Verlag, especially to Barbara Feß for perfect managing of the publication task. My thanks also go to two unknown referees for important and helpful remarks and valuable advice.

Stuttgart Günter Haag
May 2017

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Chapter 1
Introduction

Contents

The understanding of the evolution and the internal structure of our world is one fundamental stimulus of human research. We strive to find out "Was die Welt im Innersten zusammenhält" (Goethe, Faust I) and what will happen in our future or, as Douglas Adams (1979) formulated in his famous book "The Ultimate Hitchhiker's Guide to the Galaxy" in a simple but realistic way, . . .where do we come from, where do we go and where do we get the best Wiener Schnitzel?

But all attempts to understand more about issues such as the interactions of particles and molecules, the complexity of our biological world of plants, cooperation and competition of species, biological cells and the formation of organs in the fields of physics, chemistry and biology or in the social sciences the dynamics of economic and social conflicts, decision making, opinion formation and group dynamics, the building of networks, of urban and regional systems, the traffic dynamics and collective phenomena in the election of political parties—all these issues are based on models.

Models can be formulated and built in different languages. In agriculture, there exists a long tradition of farmers, applying models based on hundreds of years of experience, condensed in country sayings and weather proverbs. Meteorology formulates models for weather forecasting in the language of physics and mathematics. Models are based on rules. Rules are based on experience and experiments. The aim of modelling is always to develop a mathematical model as an image or picture of reality, formulated in logical symbols instead of words and rules representing the interactions of the symbols. This means we share the viewpoint of John L. Casti (1992a, b) "The study of natural systems begins and ends with the specification of observables describing such a system, and a characterization of the manner in which these observables are linked".

The model builder has always the choice what to observe and use as input and what to ignore. In other words, to neglect things deemed irrelevant for the purpose

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of the model. The model should be kept as simple as possible, said Albert Einstein, but not too simple. In other words, we are interested in the ways of model building.

The quality of a model, however, depends among others on the compliance between model output and observed data. In so far, data issues are of crucial importance for any modelling decision. The purpose is not only to detect and exclude outliers, but also to determine the quality of the data, since the quality of the data constrains the quality of the model output.

Measurement errors on one hand and uncertainties and fluctuations on the other hand are intrinsic in all experiments and data. In many applications those effects are considered as small perturbations and influence the trajectory of the system only in a marginal way. If, however, the dynamics of the system is based on nonlinear interactions, phase transitions may occur and the dynamics of the system depends on or may even be dominated by fluctuations. Since fluctuations are always present, it is natural to include them in our models right from the very beginning.

Since the fundamental work of Hermann Haken (1977, 1983), a comprehensive theory, called Synergetics for the investigation of structural self-organizing space-time features of interacting multi-component systems has been provided and has demonstrated its huge modelling potential. Although the interactions and constituting units of the various systems under consideration seem to be completely incomparable on the micro-level, a close analogy between them exists on the macro-level. The interdisciplinary universality of Synergetics has its origin in the unifying concepts of model building and classification of such phenomena.

In the natural sciences, the elementary units, such as atoms or molecules, and the fundamental interactions, constituting the system are generally well known. In principle, model assumptions can directly be verified or falsified by experiments, and the reproducibility of experiments is fundamental and constitutive. Typically, one and the same experiment has to be and can be repeated under identical conditions in order to measure the value or the statistical distribution of values of an observable with a definite precision.

Much research has been done investigating self-organizing phenomena in the field of physics, chemistry and biology (Weidlich 1972; Schuster 1984; Klüver and Klüver 2011; Mainzer 2007; Arthur 1989; Rosser 2011). In these research fields, Synergetic concepts are mainly treated on the macro-level (Weidlich 2000).

The classical or quantum mechanical density matrix formalism provides a practicable framework how ensembles of interacting particles or molecules can be treated mathematically. The huge field of cooperative phenomena provides a lot of interesting examples, such as superconductivity and ferro-magnetism, to mention a few. The statistics of the laser light, namely, the phase transition from a typical lamb with stochastically emitting atoms to the high intensity laser light, characterised by coherently emitting atoms, exemplifies a self-organizing process (Sornette 2006).

Several authors were inspired by the rich field of dynamic processes of biological systems, especially by predator prey systems (see also Chap. 6). The search for analogies between economic and biological evolution was utilised in particular by Penrose (1952), Dosi (2005), Dosi et al. (1994), and Nelson and Winter (1982). The role of technological progress as an explanation of contemporary economic growth and modelling of such highly dynamic complex processes with uncertainties are important research topics up to now. Haag (1990a, b), Pyka (1999), and Erdmann (1993) have utilized the Master equation framework to formulate a dynamic theory of decision making and an evolutionary theory of innovation. The Schumpeter Clock (Mensch et al. 1991) as a micro-macro model of economic change including innovation, strategic investment, dynamic competition and short and long swings in industrial transformation belongs to the same kind of modelling framework.

In the mid-1990s the labelling "Econophysics" (Mantegna and Stanley 1999) as interdisciplinary research field was introduced by several physicists, applying theories and methods originally developed in physics, in other disciplines like economics. Especially those research problems including uncertainty or stochastic processes and nonlinear dynamics were points of interest (Soros 1994).

A framework for modelling a wide class of socio-economic phenomena has been given in the book of Weidlich and Haag (1983). In the following, we will basically proceed along the line of argumentation given in this book incorporating the results of more recent research projects related to the field named Sociodynamics. Since the definition of all these concepts is the same as in Synergetics, one can therefore consider Sociodynamics as that part of Synergetics which is devoted to social systems (Weidlich 2006).

Coming back to the difference between natural and social sciences: in social sciences the interactions between elementary units such as individuals, households, firms are rather unknown and cannot be derived from first principles. Experimental tests repeated under identical socio-economic conditions are mostly impossible. The empirical data base related to a certain subject is often rather limited and the comparability among data sets is often not guaranteed.

In view of these differences regarding modelling of socioeconomic processes some critical remarks must be made at the beginning: firstly, no direct short-cut to transfer concepts from natural to social sciences exists. Appropriate and characteristic concepts have to be developed for the quantitative description of socio-economic processes. Secondly, Synergectics, Sociodynamics and all other concepts can be applied only under certain conditions to a specific class of genuine social phenomena (Haag 1990a, b). If these conditions are fulfilled, however, a true structural relationship between natural and social sciences and not just an accidental analogy can be found. In so far, all ingredients incorporated into the models have to come from the respective sciences to avoid physicalism, namely a direct use of physical laws and a re-interpretation of those in terms of social phenomena (Müller 2012; Vega-Redondo 2007).

We have to take into account, that the evolution of any socioeconomic system is not an autonomous process but the result of human decisions occurring over time as a broad stream of concurrent, unrelated or interrelated, individual or corporate choices. The underlying mechanisms behind the millions of decisions made every day cannot be completely controlled and influenced by public authorities, at least not in a direct way (Haag 1989). Therefore, planners in charge of such systems face the difficult task of making decisions concerning a system which is largely subject to external influences in the form of national policies and entangled economies on the one hand, while the system is influenced by decisions of private firms, investors, and other individual or corporate agents on the other hand. Only limited instruments of policy are available and at their disposal, and it is of crucial importance to know in advance which of these are likely to be most effective (Fischer et al. 1988; Ball 2012).

In so far, the human society can be regarded as a multi-component system whose members, the individuals, adopt different attitudes or kinds of behaviour (Weidlich and Haag 1983). The causes of global changes in society are assumed to be correlated with the decisions of agents to change their attitudes. A complex mixture of fluctuating rational considerations, professional activities, emotional preferences and motivations finally merge into one of relatively few well demarcated resultant attitudes. Those attitudes may be related to education, politics, economic activities and consumer habit, to mention a few. The attitude space is an open one, since hitherto unknown attitudes may develop or attitudes till now considered important may disappear.

The attitudes drive the decisions of individuals. Due to individual decision processes caused by experience, emotions and thoughts based on the individual network of personal relationships, transitions from one attitude to another one are possible.

However, the detailed micro-level describing the complex interplay of rational and emotional, conscious and subconscious, genetic and environmental influences on the decisions of individuals is typically unknown. Hence, a probabilistic description instead of a deterministic account of decision behaviour is adequate.

In thermodynamics, "entropy" is a measure of the order state of matter. In a closed system, the entropy is constantly increasing and reaches a maximum of "disorder" for its equilibrium state. Therefore, the equilibrium state represents the most probable configuration of the system. In closed physical systems there is a tendency towards increasing disorder of the micro states of the system. The relation to the probability of finding a macro state through certain micro states makes it possible to transfer the entropy concept to different areas of social science (Wilson 1970). Thus the entropy concept has in principle a probabilistic background, related to the statistical distribution of events in an uncertain situation. Numerous fields of application of the entropy concept to the modelling of socioeconomic systems have been examined, such as the distribution of commodity flows and migration flows, shopping trip distribution or traffic flow assignment. The basic idea is always that the distribution of the quantities of interest can be selected as the statistically most likely distribution by means of the entropy principle, taking into account given restrictions. With regard to the statistical foundation and analysis of spatial interaction models, we follow the fundamental theoretical work of Wilson (1970) and Nijkamp and Reggiani (1998) in Sect. 8.2. However, some criticisms of the entropy concept are also appropriate. The striking elegance of the method is limited by the necessary proximity to thermodynamics. Thus, the existence of the entropy can only be shown for equilibrium systems or systems that are close to equilibrium, that is, as long as linear regression laws apply. The treatment of systems that are out of balance, and this is often the case with socioeconomic systems, is, however, rather questionable.

The Master equation is suitable for the adequate statistical treatment of non-equilibrium states. Therefore, the probability that a certain decision configuration is realized will be introduced. The Master equation is the equation of motion for this probability distribution, where transition rates between different decision configurations are the essential constituents.

On the macro-level, in turn, the decision configuration describes the distribution of attitudes of the socioeconomic system and may be considered as an appropriate set of macro variables for the system under consideration. The modelling of such transition rates in terms of variables will turn out to be the central part of the model building in natural and social sciences, respectively.

The Master equation framework can be understood as a tool for model building, where fluctuations or uncertainties are incorporated in a systematic way. The strong model building potential of the Master equation is particularly suitable for complex systems. In other words, we consider systems consisting of many interacting sub-systems, where nonlinearities are inherent, and uncertainties or fluctuations are involved and may dominate the dynamics.

The probability distribution over a given configuration contains the most detailed information about the system. In particular, not only the mean values or sometimes the most probable values can be calculated but also higher moments such as the mean square deviations. Correspondingly, the amount of mathematics required to solve the time-dependent Master equation may be considerable. However, in most practical cases, the full information contained in the configurational probability distribution cannot be exploited due to a lack of sufficiently comprehensive empiric data. Therefore it makes sense to perform a transition to a less exhaustive description in terms of quasi-closed equations of motion for mean values and variances. These dynamic equations can be derived from the Master equation in a straightforward manner. Hence, the Master equation provides the link between the micro-level of changes of single configurations (transition rates) and the macro-level of dynamic equations of motion for mean values and variances.

The non-linear form of the quasi-closed equations of motion expresses the structure of self-consistence, which is prevalent in all socio-economic systems, namely the cyclic coupling of causes and effects.

Through their cultural and economic activities, the individual members of the society contribute to what we will call a collective field related to our society with cultural, political, religious, social and economic components. This collective field acts as an order parameter of the socio-economic system and characterizes the current phase of our society. Moreover, the collective field strongly influences the decision behaviour of the individuals, by orientating their activities. The feedback between the actions of the individuals and the collective field—the cyclic coupling between causes and effects—determines the temporal development of the system.

If the outcome of the Master equation, the probability distribution function, is sharply peaked, a quasi-stable temporal development of the system characterized by a certain predictability of its trajectories may occur. However, highly divergent alternative paths of evolution of the society are possible, if the control parameters of the system attain certain critical values. Fluctuations on the micro-scale may decide into which of the divergent paths the society will bifurcate. The actions of a few influential persons or decision makers could be an example. In this case, the probability distribution for the decision configuration has lost its simple uni-modal structure (Haag 1989). Nearby the phase transition point, forecasting the system development is rather difficult if not impossible.

On the macro-level phase transitions may lead to stable attractors, periodic structures, limit cycles or even chaotic trajectories. An excellent introduction into the field of chaotic systems is given by Devaney (2003) and Gollub and Baker (1996).

In social sciences, the link between the micro-level of decisions of individuals and the macro-level of the dynamics of aggregated variables is one main target of research. However, this important link is not only of theoretical interest. It enables us to match empirical data with the outcome of the theoretical model. Of course, it is well known in this context, that it is difficult if not impossible, to give a direct and unique causal interpretation of the socio-economic situation and the behaviour of certain macro-variables of society in terms of individual motivations on the micro-level (Coleman 1992). Instead, we expect that many combinations of such motivations will merge with different intensities in the individual decision processes and will produce the observed macro-dynamics. This favours the introduction of aggregated variables (e.g. attractiveness variables), which themselves depend on a set of individual motivations.

The estimation of the parameters of the model, denoted as trend parameters, is a further important research topic in social sciences. Depending on the research issue, it is sometimes possible to introduce a cost function or penalty function, which can be used to minimize the deviations between the empirical data and the model output, taking into account various constraints. Different solution algorithms can be developed and used to optimize the parameter estimation process. In Chap. 8, we will deal with these problems.

The book is organized in three parts (see Fig. 1.1):

Part I contains the statistical fundamentals and the derivation of the Master equation and the Fokker-Planck equation. Solution methods of the Master equation, including some rather new tools for a group of special problems are presented. This part is rather technical and can be used as a toolbox.

In Chap. 2, some statistical fundamentals needed for the understanding of the modelling framework of the Master equation are presented. This includes the definition of common statistical indicators and functions. This tool box is important since stochastic processes are becoming increasingly important in many branches of physics, chemistry, biology, population dynamics, economics and social sciences. Despite the diversity of tasks and problems in these fields, there are common principles and methods which are subject of this book.

Chapter 3 is concerned with the general understanding of the fundamental aspects of the Master equation. Following the introduction of some concepts of probability theory, the Markov assumption is introduced and the Chapman-Kolmogorov

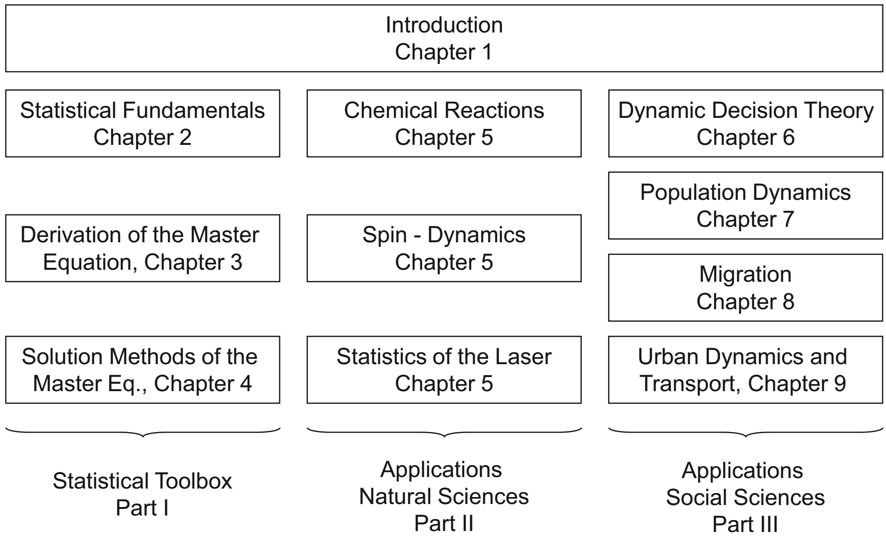

Fig. 1.1 Organization of the book

equation for conditional probabilities is derived. The Chapman-Kolmogorov equation serves as the starting point for the derivation of the Master equation. The derivation of general properties of the Master equation helps to understand the broad field of possible applications. The derivation of equations of motion for mean values and variances on both the stochastic and the quasi-deterministic level, using the method of shift operators completes this chapter.

After the derivation of the Master equation, it is logical to introduce and discuss different methods of its solution in Chap. 4. One obvious and frequently applied method consists in the approximate transformation of the discrete Master equation in a partial differential equation, namely the Fokker-Planck equation. The not so well known T-factor method is very efficient in the transformation of the Master equation into difference equations of reduced order and in continued fractions which are easier to handle. This method also provides a very elegant way to derive exact and approximate stationary solutions of the Master equation, even when detailed balance is not fulfilled. A general graph-theoretical method for the stationary solution developed by Kirchhoff for electrical networks is also presented. In case of detailed balance an exact solution method for the stationary probability distribution completes the tool box. The chapter closes with exact and approximate solution methods for one-dimensional Master equations with two particle jumps.

Part II starts with applications of the Master equation framework in the natural sciences. However, benchmarking of different solution methods is important in order to compare the Master equation framework with other modelling approaches. Therefore, we do not only apply the Master equation framework to different case studies, but also compare it with other solution methods.

In Chap. 5, the derived solution methods of Chap. 4 will be applied to some important applications out of the field of physics and chemistry in order to demonstrate the high potential of the Master equation approach in the field of natural sciences. Chemical reactions are typical examples of discrete dynamic processes obeying the mass action law. Since the various chemical reactions are considered independent of each other, a multinomial Poisson distribution is usually expected. However, in case of nonlinear chemical reactions we demonstrate that although the transition rates obey combinatorial mass-action law kinetics, a more complicated statistical distribution is obtained.

The investigation of the phase transition dynamics of spin-systems is used as an example in statistical non-equilibrium physics. The appearance of a ferromagnetic order from an initially disordered state, in other words the occurrence of a phase transition, in its conceptual simplicity is one reason for the interest in this widely applicable model type. The calculation of escape rates due to very large fluctuations will be investigated as well.

The derivation of the photon statistics of the Laserlight is selected as a typical quantum mechanical example out of the field of physics. The photon statistics of the Laser shows a typical phase transition at the so-called Laser threshold. The atoms of the Laser active material seem to be slaved: all atoms behave in a coordinated way and emit wave tracks in phase. It is interesting to apply the already introduced methods to this example and to learn more about how complicated discrete difference equations may be handled. Parts of this chapter are rather theoretical and may be skipped in a first reading.

Part III is dealing with modelling concepts in the social sciences. In Chap. 6, we derive a generalized dynamic choice model for interacting individuals using the Master equation approach. The famous multinomial-logit decision model is obtained when the system is in an equilibrium state and individuals are independent. The example shows that depending on the initial conditions of the system of agents (decision makers), and the strength of their interaction, quite different decision configurations may be obtained. Previous experience may also account for the decisions of agents, in other words decisions may depend on history. In this case the Markov assumption does no longer hold, and the Master equation fails. However, a simple trick seems to help: we fragment the whole time frame into small time sequences. The single time sequences are chosen so small that the Master equation holds within each time sequence, but not for the whole process. This provides a model of nested decision processes with memory. The emergence of conventions may be used as an example to underline the applicability of this method.

In Chap. 7, we deal with the issue of population growth. This is intended to point out ideas and thoughts behind the construction of models in population biology. I belief that this will help the reader to understand better the theoretical considerations and the outcome of the discrete Master equation approach compared with classical considerations in population dynamics based on assumed continuous population development. It is shown, that only if we take into account the discrete structure of the population, the complicated dynamics of the dying-out process can