Chapter 2
Background and Concepts

This work is a contribution to interweaving two lines of research that have developed in almost separate ways: Markov chains and agent-based models (ABMs). The former represents one of the simplest forms of a stochastic process while the latter puts a strong emphasis on heterogeneity and social interactions. This chapter provides an introduction to AB modeling and reviews approaches to use Markov chains in their analysis.

The main expected output of the Markov chain strategy applied to ABMs is a better understanding of the relationship between microscopic and macroscopic dynamical properties. This brings into the discussion concepts of aggregation and emergence, and it also relates to macroscopic mean-field formulations as a substantial tool in the statistical mechanics approach to social dynamics. Moreover, a series of information-theoretic tools to put the notion of levels onto mathematical grounds have been developed in recent years. A complete review of the literature dealing with these topics is clearly beyond the scope of this chapter which is rather aimed at introducing the most important concepts with reference to AB systems and Markov chains. Especially the physics-inspired approach to social dynamics has attracted a lot of interest in the last years and a huge number of papers is still produced every year. For a relatively coherent review (though, may be, no longer completely up-to-date), the reader may be referred to Castellano et al. (2009).

2.1 Agent-Based and Related Models

ABMs are an attempt to understand how macroscopic regularities may emerge through processes of self-organization in systems of interacting agents. A system at question is modeled at the microscopic level by specifying the elementary units of that system—the agents—and implementing simple rules for how these agents interact with one another. Typically implemented on a computer, the time evolution

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of such a system is computed as an iterative process—an algorithm—in which agents are updated according to the specified rules. One of the main purposes of this modeling strategy is "to enrich our understanding of fundamental processes" (Axelrod 1997, p. 25) underlying certain observed patterns, or to "explore the simplest set of behavioral assumptions required to generate a macro pattern of explanatory interest" (Macy and Willer 2002, p. 146).

One paradigmatic example of ABMs is Reynolds model of the flocking behavior of birds (Reynolds 1987). While the modeling of a flock as such is difficult, quite realistic flocking behavior is achieved if the individual birds follow simple rules of how to react upon the action of other individuals in their neighborhood. Another well-known example is Schelling's model of segregation (Schelling 1971). Here, two kinds of householders (say black and white) located on a lattice are endowed with a slight preference to settle in a neighborhood with more households of the same kind. Running that system leads to a clear spatial segregation at the global level even if the homophily preference is small. Similar effects can be observed in models of opinion and cultural dynamics, see, for instance, Axelrod (1997), Deffuant et al. (2001), Hegselmann and Krause (2002), and Banisch et al. (2010). Another paradigmatic problem that has been addressed by AB research is the emergence of a set of norms or common conventions. In the naming game proposed by Steels (1997), for instance, robots learn common word-object relations in a communication process based on trail and error. Other models in which an initial plurality in a population of agents evolves to a common consensus state include various models of opinion formation with the VM as the most simple representative (see Castellano et al. 2009 for a review of these models).

It is common to trace back the history of AB simulation to the cellular automata (henceforth CA) designed by von Neumann (1951) and later shaped by Berlekamp et al. (1982) and Wolfram (1983, 2002). And in fact, many ABMs can be viewed as a stochastic CA with asynchronous update. The methods developed in this work apply precisely to that type of models.

However, even some years before von Neumann and Ulam came up with the first CA design, another type of "individual-based" model had been introduced in a branch of theoretical biology which is today called population genetics (see Li 1977 for a collection of the seminal papers in that field). Wright and Fisher (along with Haldane known as the founders of population genetics) advocated a simple model for the evolution of allele frequencies (Wright 1932) based on microscopic assumptions of gene transmission from the parent to the children generation. In 1958, Moran (1958) made use of Markov chain theory to study a modified model and introduced what today is known as the Moran process. Later, Kimura went further in this line of research on a neutral theory of evolution with the stepping stone model (Kimura and Weiss 1964) which still later became known as the voter model (abbreviated by VM throughout this book). From the very beginning population genetics developed as a mathematical discipline and has inspired various solution strategies from probabilistic methods including Markov chains and coalescing random walks to mean-field approaches in statistical physics.

The biological literature on evolutionary dynamics on graphs has mainly started from the model proposed by Moran (1958). In the Moran model, at each time step, an individual is chosen at random to reproduce and replaces a second one chosen at random as well. In the original model, there is no population structure which means that all individuals are chosen with equal probability. Therefore—this is something that will be made explicit in the fourth chapter of this thesis—the dynamics can be formulated as a birth-death random walk on the line. See Claussen and Traulsen (2005), Traulsen et al. (2005), and Nowak (2006) for treatments of the associated Moran process. While early studies (Maruyama 1974; Slatkin 1981) had indicated that population structure has no or only little effect on the model behavior, it has recently been shown that population structure can have a significant influence (Liberman et al. 2005; Nowak 2006; Shakarian et al. 2012; Voorhees and Murray 2013; Voorhees 2013, among many others). The setting—sometimes referred to as evolutionary graph theory (Liberman et al. 2005)—is usually as follows: suppose the is a population of N individuals with fitness 1; suppose that a mutant with fitness r is introduced in one of the individuals; what is the probability that the mutant invades the entire population? The Moran case of unstructured populations is usually taken as a benchmark such that a graph which leads to a fixation probability different from the unstructured case are said to suppress or respectively enhance selection.

In the physics literature, the analysis of binary models as the VM is usually based on mean-field arguments. The system dynamics is traced in form of an aggregate order parameter and the system is reformulated on the macro-scale as a differential equation which describes the temporal evolution of that parameter. In many cases, the average opinion (due to the analogy to spin systems often called "magnetization") has proven to be an adequate choice, but sometimes the number of (re)active interfaces yields a more handable transformation (e.g., Frachebourg and Krapivsky 1996; Krapivsky and Redner 2003; Vazquez and Eguíluz 2008). A mean-field analysis for the VM on the complete graph was presented by Slanina and Lavicka (2003), and naturally, we come across the same results using our method (Sect. 4.1.2). Slanina and Lavicka (2003) derive expressions for the asymptotic exit probabilities and the mean time needed to converge, but the partial differential equations that describe the full probability distribution for the time to reach the stationary state is too difficult to be solved analytically (Slanina and Lavicka 2003, p. 4). Further analytical results have been obtained for the VM on d-dimensional lattices (Cox 1989; Frachebourg and Krapivsky 1996; Liggett 1999; Krapivsky and Redner 2003) as well as for networks with uncorrelated degree distributions (Sood and Redner 2005; Vazquez and Eguíluz 2008). It is noteworthy, that the analysis of the VM (and more generally, of binary-state dynamics) on networks has inspired a series of solution techniques such as refined mean-field descriptions (e.g., Sood and Redner 2005; Moretti et al. 2012), pairwise approximation (e.g., De Oliveira et al. 1993; Vazquez and Eguíluz 2008; Schweitzer and Behera 2009; Pugliese and Castellano 2009) and approximate master equations (e.g., Gleeson 2011, 2013).

The early works in population genetics (Fisher 1930, in particular) have inspired still another modeling approach that is related to ABMs, namely, evolutionary game theory (see Smith 1982 for a seminal volume and Roca et al. 2009 for a recent

review). Here, games are designed in which agents repeatedly play against one another adopting one out of a set of predefined strategies. A fitness is assigned to the combinations of strategies and the population evolves as a response to this fitness. As in the framework of statistical mechanics, the model evolution is typically captured in form of differential equation describing the evolution of the (relative) frequencies of the different strategies, referred to as replicator dynamics in this context (Taylor and Jonker 1978; Schuster and Sigmund 1983; Hofbauer and Sigmund 2003). One of the main purposes of this work is to spell out explicitly how to link the dynamics at the micro level to these macroscopic descriptions.

Finally, it is worth mentioning that research in economics has experienced a growing interest in modeling economic phenomena as the result of the interactions of heterogeneous individuals (Tesfatsion and Judd 2006). In particular in the field of finance, this has led to the development of ABMs for the identification of (macro) patterns of collective dynamics from (micro) investor heterogeneity in many financial settings (Cont and Bouchaud 2000; LeBaron 2000; Bornholdt 2001; Kaizoji et al. 2002; Hommes 2006; Preis et al. 2013; Krause and Bornholdt 2013; Patzelt and Pawelzik 2013). Noteworthy, there is also a number of empirical applications of Markov chains in the field of finance (e.g., Corcuera et al. 2005; Nielsen 2005; Norberg 2006). Interaction and heterogeneity on the one hand, and non-Gaussianity, heavy tails and long-range correlations on the other appear to be natural features of modern economies, to which the formerly dominating tradition of modeling representative agents has, to a large extent, paid little attention. This thesis shows that memory effects at the macroscopic level are an immediate consequence of microscopic heterogeneity and it may therefore contribute to the identification of the relevant microscopic mechanisms that presumably play a role in the market.

2.2 Markov Chain Formalization of Agent-Based Models

The AB approach is first and foremost a computational methodology and the mathematical formalization of the models is in its infancy. This is probably due to the fact that a major motivation in the development of AB simulation has been to relax a series of unrealistic assumptions made in other modeling frameworks just in order to keep mathematical tractability; namely, rationality, perfect information, agent homogeneity, and others. The other side of the coin is that the focus on computer models and algorithms makes difficult the comparison of different models and also complicates a rigorous analysis of the model behavior. In fact, the problems of code verification and model comparison including the discussion of standards for the replication of ABMs has nowadays become an area of research in its own (e.g., Axtell et al. 1996; Axelrod 2003; Hales et al. 2003; David et al. 2005; Grimm et al. 2006; Wilensky and Rand 2007; Galán et al. 2009). As a matter of fact, many of those problems would actually vanish with a sound mathematical formulation of an AB simulation model. On the other hand, it is also clear that the precise mathematical specification of a high-dimensional system of heterogeneous

interacting agents along with their update mechanisms can be cumbersome in more complex models.

To the authors knowledge, the first systematic approach to the development of mathematical formalism for ABMs in general is due to Laubenbacher and co-workers. Laubenbacher et al. (2009) review existing formal frameworks that have the potential to model AB systems, such as cellular automata and finite dynamical systems and argue for the latter as an appropriate mathematical framework to represent ABMs. However, the probabilistic nature of most models can only be accounted for by the stochastic version—the so-called stochastic finite dynamical systems—the analysis of which "is still in its infancy" (Laubenbacher et al. 2009, p. 14). On the other hand, Laubenbacher et al. (2009) recognize that stochastic finite dynamical systems give rise to Markov chains. However, for reasons that do not become very clear in their paper, the authors argue:

> To understand the effect of structural components such as the topology of the dependency graph or the stochastic nature of the update, it is important to study them not as Markov chains but as SFDS [stochastic finite dynamical systems] (Laubenbacher et al. 2009, p. 10)

I clearly disagree with them in this point, because the microscopic specification of ABMs as Markov chains developed in this thesis turns out to be a useful starting point for further analysis. But of course, the incentive of Laubenbacher et al. (2009) to further elaborate the theory of stochastic dynamical systems in order to derive rigorous results for ABMs in future is highly appreciable.

The usefulness of the Markov chain formalism in the analysis of ABMs has first been realized by Izquierdo et al. (2009). The authors look at ten well-known social simulation models and discuss for each of them how to represent the model as a time-homogeneous Markov chain. Among the models studied in Izquierdo et al. (2009) are the Schelling segregation model (Schelling 1971, for which some analytical results are available, for example, in Pollicott and Weiss 2001; Grauwin et al. 2010), the Axelrod model of cultural dissemination (Axelrod 1997, see also Castellano et al. 2000 for a mean-field approximation) and the sugarscape model from Epstein and Axtell (1996). Noteworthy, the sugarscape model—one of the reference models in the field of social simulation—contains virtually all features that may occur in ABMs: heterogeneous agents placed in a dynamic spatial environment, death and birth of agents, various static and dynamic attributes that may evolve on different time scales.

The main idea of Izquierdo et al. (2009) is to consider all possible configurations of the system as the state space of a huge Markov chain and the construction of that state space is actually the main challenge for Izquierdo and co-workers. Despite the fact that all the information of the dynamics of the ABM is encoded in a Markov chain, however, it is difficult to learn directly from this fact, due to the huge dimension of the configuration space and its corresponding Markov transition matrix. The analyses provided in Izquierdo et al. (2009) are essentially based on the classification of states into transient and absorbing communicating classes which allows some statements about the convergence as times goes to infinity.

The paper of Izquierdo et al. (2009) is designated "for researchers who may not have a strong mathematical background" (par.1.1) and probably therefore lacks rigorous arguments sustaining some of the results. Most fundamentally, there is no proof that the process on the constructed configuration space indeed satisfies the Markov property. Their work also mainly relies on numerical computations to estimate the stochastic transition matrices of the models. Both issues are addressed in this volume. The explicit computation of transition probabilities, in particular, allows for the application of the theory of Markov chain aggregation in order to reduce the state space of the model.

2.2.1 A Very Short Introduction to the Markov Chain Setting

For the purposes of this book, it is not necessary to provide an extensive overview of Markov chain theory. It is more convenient here to introduce the general idea for using Markov chains for the representation of ABMs and introduce the analysis tools of Markov chain theory when we apply them to the models. In Chap. 4, for instance, we will analyze the voter model on the complete graph which gives rise to an absorbing birth-death process known as Moran process (Moran 1958). The standard tools for the analysis of absorbing chains are introduced and applied there. In the same way Chap. 6 can be consulted for the analysis of regular Markov chains. In the applications of Markov chain tools presented throughout this book we mainly follow Kemeny and Snell (1976), Behrends (2000), and Levin et al. (2009). Many other volumes (introductory and advanced) are available.

Here we concentrate on ABMs with a finite number of agents that are characterized by a finite set of discrete attributes. This means that the state space of the system—that is, the set of all possible system configurations—is also finite.[1] It will be denoted as Σ in the sequel. Furthermore, AB simulation models usually implement time-discrete processes and due to these ingredients taken together we concentrate on finite-state, discrete-time processes.

A Markov chain is a stochastic process in which the probability to observe a state $\mathbf{y}$ at time $t+1$ is completely determined by the preceding state $\mathbf{x}$ at time t. It is common to express this in form of a transition probability matrix $\hat{P} : \Sigma \to \Sigma$ that contains the transition probabilities for all pairs of states $\mathbf{x}, \mathbf{y} \in \Sigma$. Then, considering a initial distribution $\hat{\pi}(0)$ that assigns an initial probability to all the possible system states, the time evolution is given by the repeated application of the transition matrix $\hat{\pi}(t) = \hat{\pi}(0)\hat{P}^t$ where $\hat{\pi}(t)$ now contains the probability for the system states at time t.

[1] Notice, that this excludes a series of models (e.g. continuous opinion dynamics Deffuant et al. 2001; Hegselmann and Krause 2002) that operate with agents characterized by a continuous variable.

Throughout this book, we will mainly be confronted with two different classes of Markov chains, namely, absorbing and regular chains. This first ones are characterized by the fact that there are certain states $\mathbf{x}$ in the system with no outgoing probabilities, meaning that the system will remain in $\mathbf{x}$ once it has entered it. In other words, $\hat{P}(\mathbf{x}, \mathbf{x}) = 1$ and the process is said to converge to the absorbing state $\mathbf{x}$. For this reason, questions concerning convergence times and the number of times the non-absorbing, transient states are visited before convergence are among the most interesting. As already mentioned, the tools to address those questions are introduced in Chap. 4.

Regular chains, to the contrary, are characterized by the fact that there is a certain time t at which the matrix $\hat{P}^t$ has only positive elements. This obviously excludes absorbing states as the respective outgoing transition probabilities for these states will always remain zero. It basically means that in regular chains every state can be reached from every other state in the course of the process. Moreover, the powers of the transition probability matrix approach a limiting matrix for $t \to \infty$ in which all rows are the same probability vector. Therefore, independent of the initial distribution $\hat{\pi}(0)$, a regular chain always converges to a fixed probability vector $\hat{\pi}$ which is called the stationary distribution of the chain. Since the stationary vector $\hat{\pi}$ is constant under further application of the transition matrix, one way to compute this vector is solve the eigenvalue problem $\hat{\pi}\hat{P} = \hat{\pi}$ (for the eigenvalue 1). Chapter 6 will deal with an ABM that gives rise to regular chains.

When simulating an ABM, one usually initializes the system with particular (often random) initial assignments of the agent attribute corresponding to one specific system configuration $\mathbf{x}$. The initial distribution corresponds in this case to a vector that contains zero everywhere except for the element representing $\mathbf{x}$ where it is one (i.e., $\hat{\pi}_{\mathbf{x}}(0) = 1$ and $\hat{\pi}_{\mathbf{y}}(0) = 0, \forall \mathbf{y} \neq \mathbf{x}$). However, in order to understand the dynamics of a model, a series of numerical experiments is usually performed each with a different initial condition. This can be accounted for by setting $\hat{\pi}$ accordingly. One of the strength of using Markov chains is then that the statistics one derives from the analysis accounts for the statistics that would be observed for infinitely many model realizations.

2.3 Lumpability and State Space Aggregation

The state space of a Markov chain derived by considering as states all possible system configurations is far too big to directly use the respective transition matrix $\hat{P}$ for exact numerical computations. As an example, consider a model with binary agent attributes such as the VM. A system of N agents will lead to a Markov chain of size 2^N which for our introductory example of only 20 agents (Fig. 1.1) leads to a chain with more than a million states. In order to use the Markov chain machinery for AB systems, the system size has to be reduced in some way.

2.3.1 Strong Lumpability

This brings lumpability into play as a way to combine and aggregate the states of a Markov chain so that the process at the aggregate level is still a Markov chain. Consider that the state space of a Markov chain is Σ and the transition probabilities between all pairs of states in Σ are given by the $|\Sigma| \times |\Sigma|$ transition matrix $\hat{P}$. Throughout this work, the chain $(\Sigma, \hat{P})$ will be called micro chain and, respectively, the states in Σ micro states. Now assume that $\mathbf{X} = (X_0, X_1, \ldots, X_n)$ is a partition of Σ where each X_k contains a set of micro states in Σ, such the X_k are disjoint ($X_k \cap X_s = \emptyset$ for any pair of aggregate sets) and for the union of all sets $\bigcup_{i=0}^{n} X_i = \Sigma$. Such a situation naturally arises if the process is observed not at the micro level of Σ, but rather in terms of a measure on Σ, $\phi : \Sigma \to \{0, 1, \ldots, n\}$, by which all states in Σ that give rise to the same measurement are mapped into the same aggregate set X_k (also referred to as macro states). An important question that arises in such a setting is whether the new aggregate process on $\mathbf{X}$ is still a Markov chain or not. This is what lumpability is about. The lumpability theory adopted for the purposes of this thesis is largely based on Kemeny and Snell (1976), which is, to the authors knowledge, the first textbook in which the strong as well as the weak form of lumpability are discussed with some detail. Notice that there are some other early and seminal works on lumpability, such as Burke and Rosenblatt (1958), Rosenblatt (1959), and Rogers and Pitman (1981).

To illustrate the concept of *strong lumpability*, let us use the Land of Oz example repeatedly considered in Kemeny and Snell (1976) (see pages 29/30 for the introduction of the example and page 125 for the lumpability example). There, a three-state Markov chain is formed which approximates how the whether develops from 1 day to the other. There is rain (R), nice whether (N) and snow (S) and the transition rates are given by

$$\hat{P} = \begin{matrix} R \\ N \\ S \end{matrix} \begin{pmatrix} 1/2 & 1/4 & 1/4 \\ 1/2 & 0 & 1/2 \\ 1/4 & 1/4 & 1/2 \end{pmatrix}. \tag{2.1}$$

Therefore, a nice day is never followed by a nice day, but there is an equal chance to have rain or snow. For a rainy day as well as for a day with snow, on the contrary, there is a chance of $1/2$ that the whether remains as it is for the next day, and the remaining options are equally likely with probability $1/4$. From this assignment of probabilities, we can already see that the behavior for rain (R) and snow (S) is actually equal and therefore we may combine the two states into a "macro" state called "bad whether" ($B = \{R, S\}$). Hence, the states space is partitioned into two sets: N on the one hand and $B = \{R, S\}$ on the other. Now, as the probability that nice whether follows is equal for R and S the transition matrix of the new chain is uniquely defined by:

$$P = \begin{matrix} N \\ B \end{matrix} \begin{pmatrix} 0 & 1 \\ 1/4 & 3/4 \end{pmatrix}. \tag{2.2}$$

It is the equality of conjoint transition rates from the states that shall be combined to all the other partitions ($\hat{P}(R,N) = \hat{P}(S,N) = 1/4$ in this simple example) on which the condition for lumpability is based.

More precisely, if the probability of moving from a micro state $\mathbf{x} \in X_k$ to a macro state X_l is equal for all micro states in X_k, then all the information about the history which led to a particular state in X_k is actually irrelevant, because from the macro perspective the future evolution is equivalent for any state in X_k. This leads to a condition on the transition matrix $\hat{P}$, namely, $\sum_{\mathbf{y}\in X_l} \hat{P}(\mathbf{x} \in X_k, \mathbf{y} \in X_l)$ must be equal for all $\mathbf{x} \in X_k$. For a process to be lumpable with respect to a partition $\mathbf{X}$, it is sufficient and necessary if this is true for any pair of sets X_k, X_l of the partition. The respective theorem is presented in Kemeny and Snell (1976, Theorem 6.3.2) and we will come back to it with more detail and a focus on an application to ABMs in Sect. 3.3.3 (next chapter).

If the chain along with the desired state space partition is given, the application of the conditions provided in Kemeny and Snell (1976, Theorem 6.3.2) (as well as the subsequent matrix conditions) is relatively simple. However, if only the chain is given, it may be a real challenge to find partitions with respect to which the process is lumpable, not least due to the combinatorial explosion of the number of possible partitions. In this context, some algorithms have been presented for the task to find the optimal or coarsest partition (Buchholz 2000; Derisavi et al. 2003). Other authors have addressed these issues by studying the spectral properties of lumpable chains and have proposed algorithms based on that (Barr and Thomas 1977; Meila and Shi 2001; Takacs 2006; Jacobi 2008; Filliger and Hongler 2008; Görnerup and Jacobi 2010).

Another approach in which aggregate Markov chain descriptions are derived on the basis of model specifications that include the hierarchical and symmetric composition of sub-models has been followed by Buchholz (1995) and is also advised in the context of interactive Markov chains by Hermanns (1999) and Hermanns and Katoen (2010). Namely for systems that "include a large number of identical and symmetric components" (Buchholz 1995, pp. 93/94), a reduced Markov chain description "resulting from exact lumping" (Buchholz 1995, p. 94) is constructed directly during the modeling process. This avoids time-consuming (up to unfeasibility) computations on the huge transition matrices that the model would give rise to without the reduction. In this work, we formulate explicitly the complete microscopic system—containing all symmetries that come by the ABM at question—and lumpability arguments are based on that description (Sects. 3.2 and 3.3, next chapter). However, one of the main messages of this work concerns the translation of model symmetries into regularities on the associated micro chain which then enable lumpability. Especially Chap. 5, in which aggregate descriptions are derived starting from the symmetries of the agent network, is clearly related to the hierarchical approach due to Buchholz (1995) and the idea of symmetric composition in Hermanns (1999).

2.3.2 Weak Lumpability

This thesis mostly applies the strong version of lumpability described above in order to achieve a Markovian aggregation for ABMs. However, it is important to note that there is a weaker version of lumpability often referred to as *weak lumpability* which will play some role in the seventh chapter. While in the case of strong lumpability the projected process on $\mathbf{X} = \{X_0, X_1, \ldots\}$ is a Markov chain for any (initial) distribution, the weaker form of lumpability makes statements about the possibility to obtain a Markovian process at the aggregate level only for particular initial vectors.

For a description of the intuition behind weak lumpability the reader is encouraged to have a look to Kemeny and Snell (1976, Sect. 6.4., and pages 132/133 in particular) who themselves refer to Burke and Rosenblatt (1958) for some of their results. The main idea resides in the following possibility:

> Assume that no matter what the past information is, we always end up with the same assignment of probabilities for being in each of the states in $[X_k]$. Then again the past can have no influence on our predictions. (Kemeny and Snell 1976, p. 133)

A necessary and sufficient (though not always practical) condition (Kemeny and Snell 1976, Theorem 6.4.1) is also provided, but the necessity and sufficiency of conditions for weak lumpability have also been subject of further discussion, see Abdel-Moneim and Leysieffer (1982), Rubino and Sericola (1989), and Peng (1996).

On of the most important observations concerns the fact that if a regular chain is weakly lumpable with respect to a partition $\mathbf{X}$ for some probability vector, then it is weakly lumpable for the stationary vector (the left invariant vector of the transition matrix $\pi P = \pi$). See Kemeny and Snell (1976, Theorem 6.4.3) and also Rubino and Sericola (1989). This may be useful for the decision whether there is one distribution altogether for which a chain is weakly lumpable or not (Kemeny and Snell 1976, Theorem 6.4.4). This result has been extended to absorbing Markov chains by Ledoux et al. (1994). In the absorbing case, the quasi-stationary distribution is shown to play the role of the stationary vector which allows to relate the lumpability problem and existing algorithms for irreducible chains to the absorbing case.

2.3.3 Nearly Lumpable and Non-lumpable Aggregation

It is well known that lumpability (the strong as well as the weak version) is rather an exception than the rule (Chazottes and Ugalde 2003; Gurvits and Ledoux 2005). Some form of aggregation, state space reduction, or macroscopic observation, however, is omnipresent in the analysis of complex systems and their dynamics. The question that then arises concerns the extend to which an aggregate process still informs us about the real microscopic model behavior.

There are some works that discuss these issues for the cases that the aggregation satisfies different types of lumpability. Namely, Schweitzer (1984), Sumita and Rieders (1989), and Buchholz (1994) show that important stationary and transient measures are preserved by the lump. However, the direct derivation of stationary and transient properties of the original chain only by knowledge of the aggregated chain is possible only for a special case of weak lumpability referred to as *exact lumpability* (Buchholz 1994, Theorem 3, Theorem 6). Buchholz (1994) also states that for any micro process and any partition it is possible to construct an aggregation that preserves the stationary measure. However, for the construction of this so-called *ideal aggregate* the stationary state of the original micro system has to be known. Though all lumpable aggregation are also ideal, the converse is not true and Buchholz (1994, p. 6) states:

> In all cases considered here, no information about the transient behavior can be gained from the ideal aggregate.

In Chap. 7 of this work, we will construct an ideal non-lumpable aggregate for the contrarian VM on networks. While this book does not go much further in analyzing the relation between that ideal aggregate and the micro process, it does present an analytical example in which these questions can be addressed.

A second important contribution due to Schweitzer (1984) and Buchholz (1994) is an operational concept of *near lumpability*. The main idea is that a nearly lumpable transition matrix $\hat{P}$ can be represented as $\hat{P} = \hat{A} + \epsilon\hat{B}$ where $\hat{A}$ is lumpable and ϵ is a sufficiently small constant used in analogy to its use in perturbation theory. Buchholz (1994) constructs bounding matrices for the transition probabilities that can be used to compute bounds for the stationary and transient quantities of the aggregated process. The computation of bounds in Buchholz (1994) is in part based on the work of Courtois and Semal (1984). See also Franceschinis and Muntz (1994) and Dayar and Stewart (1997) for other concepts of nearly- or quasi-lumpability.

2.3.4 Aggregation in Dynamical Systems

Finally, to complete this section, we should notice that aggregation and state space decomposition is a wide field which has been vividly discussed across different disciplines, during quite some time. In philosophy, it relates strongly to the more general discussions about the decomposability of a complex system (Simon 1962) and from there to emergence (Wimsatt 1986; Auger and Poggiale 1998) and even further to the possible limitations of an reductionist account of complex systems (Wimsatt 2006a). In economics, where much theory is in fact developed around aggregate measures, techniques for the aggregation of variables in dynamical systems have been developed (e.g., Theil 1965; Simon and Ando 1961; Ando and Fisher 1963) as an operationalization "decomposability" and "nearly-decomposability" of a complex system mentioned above (Simon 1962). These techniques have been transferred to theoretical biology, ecological modeling and

population dynamics in particular, by Iwasa et al. (1987) in which conditions for exact aggregation in non-linear dynamical systems are given and Iwasa et al. (1989) which deals with approximate aggregations. The fact that the explicit consideration of more and more factors is a tendency in modern model development, has led to a renewed interest in aggregation techniques not only in Markov chains but also in the context of dynamical systems (see Auger et al. 2008 for a review of aggregation methods with application to population dynamics).

It is clear that aggregation techniques are actually relevant to all models which involve a large number of variables (or agents), in order to derive reduced model descriptions that might be amenable to analytical strategies. Markov chains and dynamical systems are probably the two most important mathematical formalisms to represent complex and high-dimensional systems that evolve in time. In this context, it is very interesting that methods for aggregation of variables in linear dynamical systems and lumpability in Markov chains can be based on the same principles, a fact that has recently been exploited in Jacobi and Görnerup (2009) and Görnerup and Jacobi (2010).

2.4 The Information-Theoretic Perspective

A useful complementary view on lumpability and state space aggregation more generally is provided by a series of information-theoretic approaches that are recently developed in the context of multi-level dynamical systems (Shalizi and Moore 2003; Görnerup and Jacobi 2008, 2010; Jacobi and Görnerup 2009; Pfante et al. 2014a,b). Albeit being applied to dynamical systems more generally, the setting is strongly related to the questions of lumpability in Markov chains. Consider a Markov chain $(\Sigma, \hat{P})$ with state space Σ and a transition matrix $\hat{P}$ and an operator $\phi : \Sigma \to \mathbf{X}$ that projects the system onto a higher-level coarse-graining $\mathbf{X}$ of Σ inducing a dynamical process on $\mathbf{X}$. The question of lumpability is basically whether the induced process on the $\mathbf{X}$-level is still Markovian.

In the previous section, we have somehow considered that the partition $\mathbf{X}$ is already defined. This is reasonable in many cases, for instance, in most AB studies where the system property one wishes to analyze defines a projection (see Chap. 3). However, in multi-level systems more generally, the state space partition $\mathbf{X}$ might not be known beforehand. This leads to questions of level-identification where one has to find projection operators (and consequently partitions) that lead to a "closed" description (at least approximately), in the sense that the system can be modeled by the state variables of this level. Information-theoretic measures can be used in order to quantify "closedness", or, to be precise, deviations from it. Here we shall mention three of these measures:

Markovianity Shalizi and Moore (2003) emphasize the particular role of Markovianity in the definition or identification of macroscopic observables. Based on that, Görnerup and Jacobi (2008) propose a Markovianity measure following the

idea that an higher level is closed if the dynamic $P : \mathbf{X} \to \mathbf{X}$ induced at this level is Markovian. The decision whether the macro process (obtained by a certain projection) is Markovian or not is based on the mutual information between the past $(\ldots, X_{t-2}, X_{t-1})$ and the future $(X_{t+1}, X_{t+2}, \ldots)$ with respect to the present (X_t). If the expected mutual information between past and future is zero, looking further back into the past does not provide any new information about the future evolution, that is, the future depends only on the present value X_t and the sequence induced at the macro level is a Markov process. In other words, the conditional past-future mutual information $I(X_{t+1}; X_{-\infty}^{t-1} | X_t)$ vanishes. Noteworthy, they show that their Markovianity measure can be expressed in terms of the slope of block entropies which bears a relation to process reconstruction in turbulence and finance (Chazottes et al. 1998; Vilela Mendes et al. 2002).

Informational Closure According to this measure, introduced in Pfante et al. (2014a), a level is informational closed if the knowledge of the micro-level state $\mathbf{x}_t$ at time t does not allow for better predictions of the macro level X_{t+1} than the knowledge of the preceding macro state X_t. This can be written as the conditional mutual information $I(X_{t+1}; \mathbf{x}_t | X_t)$ which quantifies the information flow from the original to the higher level. In other words, this measure quantifies micro-level information that a higher-level description does not account for and consequently a level is closed if $I(X_{t+1}; \mathbf{x}_t | X_t)$ vanishes. As shown in Pfante et al. (2014a), $I(X_{t+1}; X_{-\infty}^{t-1} | X_t) \leq I(X_{t+1}; \mathbf{x}_t | X_t)$ so that vanishing information flow from micro to macro implies Markovianity. Moreover, in most situations information flow can distinguish between the strong and the weak form of lumpability as it vanishes for the former but not for the latter.

Predictive Efficiency The intuition behind predictive efficiency, introduced in Shalizi (2001) with important predecessors in Grassberger (1986), Lindgren and Nordahl (1988), and Crutchfield and Young (1989) (among others), is that a coarse-grained description with state space $\mathbf{X}$ can be considered as a level if it is informative for the dynamics at this level while, at the same time, being not too complex. Shalizi (2001) introduces the notion as the ratio between excess entropy and statistical complexity and uses it to define emergent processes. Based on this, two variants of predictive efficiency are introduced in Pfante et al. (2014b): first, the ratio $I(X_{t+1}; X_t)/H(X_t)$ between one-step mutual (prediction) information and the entropy of the description; second, the variational $I(X_{t+1}; X_t) - \beta H(X_t)$ which relates the measure to the information bottleneck method (Tishby et al. 1999).

We will come back to these measures in the seventh chapter where we study a non-absorbing variant of the VM on a two-community graph. The projection of the micro dynamics of this model onto the macroscopic level is not lumpable which means that memory effects are introduced in the transition from the micro to the macro level. For the special two-community case we are able to compute Markovianity and informational closure explicitly.

The information-theoretic setting described in this section is also related to the framework of computational mechanics (Crutchfield and Young 1989; Shalizi and Crutchfield 2001; James et al. 2011, and references therein). The main idea

in computational mechanics is to group histories which give rise to the same conditional probability distribution over futures into equivalence classes—so-called causal states—and to construct in this way a minimal causal model—called ϵ-machines—for the prediction of the process at question. The reader may be referred to Shalizi and Crutchfield (2001) for an overview and several interesting theoretical results in computational mechanics. The applicability of these measures to AB and related computational models is limited by their computational complexity (cf. Görnerup and Jacobi 2008, p. 13). The fact that, even in very simple ABMs, the state space of the process to be handled becomes very large challenges these approaches in two ways. The first one concerns the "combinatorial explosion" (Görnerup and Jacobi 2008, p. 11) of the number of possible partitions, which is a general difficulty for level identification where the partition is not given a priori. Secondly, the larger the alphabet, the more data must be generated and evaluated in order to obtain a workable approximation of the joined probability distribution of sequence blocks (cf. Shalizi and Crutchfield 2001, Sect. VII.B/C). One way to deal with this problem is to restrict to block size to one, as in Shalizi et al. (2004), which is actually exact if the original process is a Markov chain. Still, in this case, the number of states is huge and the estimation of the conditional probabilities (on the basis of which equivalence classes are constructed) requires a lot of simulation data.

2.5 Motivation: Towards a Markov Chain Theory of Aggregation for Agent-Based Models

2.5.1 Bridging a Gap

Though it has often been recognized that ABMs may be conceived as (stochastic) dynamical systems or Markov chains (Epstein and Axtell 1996; Laubenbacher et al. 2009; Izquierdo et al. 2009; Page 2012), the afore mentioned aggregation techniques developed for these systems have not yet been applied to ABMs. One of the reasons for this is that an explicit formulation of the micro process in terms of dynamical systems or Markov chains has been accomplished only in an abstract (Laubenbacher et al. 2009; Page 2012) or approximate (Izquierdo et al. 2009) way. The explicit formalization of the micro process as a Markov chain—the reasoning presented in this book will be started with it (Sect. 3.2)—enables the application of the Markov chain theory of aggregation—that is, lumpability—to ABMs.

The need for a mathematical framework that links the micro and the macro level has, of course, been noted earlier. For instance:

> Of course, microscopic and macroscopic theories are related, and understanding the connection between the two, e.g., through simulation or by deriving the latter from the former, is an important goal of any complex systems research. (Lerman 2001, p. 225)

Also the general possibility of applying mathematical aggregation techniques (Page 2012) and complexity reduction by symmetry exploitation (Laubenbacher et al. 2009) has been noted, namely, in the context of dynamical systems and partly based on earlier work by Iwasa et al. (1987) in population ecology. However, a sophisticated and practicable mathematical framework for linking between micro and macro level processes in an AB system does not yet exist. This work is a first step to bridge this gap.

2.5.2 The Micro-Macro Link

The relation between the microscopic and the macroscopic has since long been subject for controversy. In sociology, it is manifest in the dichotomy of methodological individualism and structural functionalism. A good overview over the historical development of micro-macro debates from philosophy to social theory is provided in the introductory chapter (Alexander and Giesen 1987) of a volume headed "The Micro-Macro Link" (Alexander et al. 1987).

"The Micro-Macro Link" is a collection of essays by very influential social theorists in the micro as well as in the macro tradition about ways to overcome the micro-macro divide and link between the different levels of analysis. A synthetic formulation embracing the different levels from individual action to social order and back requires on the one hand a link from the micro to the macro pointing at questions related to various (from weaker to stronger) forms of emergence (Brodbeck 1968; Giesen 1987), aggregation and equilibrium (Coleman 1987). On the other, it should also include concepts for the retro-action of the macro on the micro level, such as internalization (Parsons 1954) or constraints on and the environment of individual actions (Alexander 1987). One of the first acknowledged synthetic formulations of this linkage between micro and macro in sociology studies is from Max Weber (1978) from where we quote the following basic observation:

> within the realm of social action, certain empirical uniformities can be observed, that is, courses of action that are repeated by the actor or (simultaneously) occur among numerous actors (Weber 1978, p. 29)

We shall see how a stylized version of this belief is incorporated in our study when passing from micro to macro dynamics.

AB simulation is sometimes considered as a methodology to provide a "theoretical bridge" (Macy and Willer 2002, p. 148) between micro and macro theories (see also Saam 1999; Squazzoni 2008). Even if most of the models (especially the early ones) are actually a straight implementation of the individualistic program, there are some attempts to include into the model agents with some socio-cognitive abilities (see Squazzoni 2008, pp. 14–16) capable of the perception and internalization of the macro sphere. Also the experimentation with different interaction topologies can actually be seen as an attempt to understand the influence of social structure

(macro) on the emergence of collective order (macro) transmitted through the level of individual interaction (micro).

Clearly, this book is not about social theory. It is about a mathematical technique to link micro dynamics to macro dynamics in models that may be designed on the basis of sociological theorizing. To my opinion, a well posed mathematical basis for these models may help the understanding of many of their observed properties, and it also provides a new perspective on aggregation and emergence and on how they are related. Linking the micro-description of an ABM to a macro-description in the form of a Markov chain provides information about the transition from the interaction of individual actors to the complex macroscopic behaviors observed in social systems. In particular, well-known conditions for lumpability (Sect. 2.3.1) make it possible to decide whether the macro model is still Markov. Conversely, this setting can also provide a suitable framework to understand the emergence of long range memory effects and patterns of spatial organization (Chap. 7).

2.5.3 Computational Emergence and Aggregativity

ABMs and other related computational tools (such as CA) play an increasingly important role also in the contemporary philosophical discussions of emergence. Some philosophers (e.g., Bedau 1997, 2003; Huneman and Humphreys 2008; Humphreys 2008) advocate a position which makes use of computational models as a playground to address fundamental questions of emergence (see Symons 2008 for a critical consideration). Questions about the relation of these artificial model environments to real phenomena are not ignored, but considered as an independent issue which is actually part of another debate. The field of computational emergence aims to establish "a close link between the concept of emergence and computation or computer simulations, which can perhaps be captured by the idea that an emergent phenomenon is one that arises from a computationally incompressible process" (Huneman and Humphreys 2008, pp. 425/426). The framework presented here provides explicit knowledge about the (in)compressibility of computational models and the dynamical processes which these models give rise to.

While scientists use the term "emergence" relatively freely, the philosophical literature differentiates more carefully between different forms of emergence (ontological versus epistemological, strong versus weak, synchronic versus diachronic emergence) and the existence of some of these forms (ontological emergence in particular) is in fact highly controversial. In the context of computational models, emergence is often paraphrased by "the whole is more than the sum of its parts" and an emergent property can be a certain macro-level pattern that could not be expected (and not predicted!) by looking at the micro level rules only. Along this lines, a well-known and explicitly computational account of weak emergence that fits the use of the term in complexity science has been offered by Bedau (1997, 2003):

> The behavior of weakly emergent systems cannot be determined by any computation that is essentially simpler than the intrinsic natural computational process by which the system's behavior is generated. (Bedau 2003, p. 18)

Bedau (2003) uses CAs to illustrate these ideas and makes explicit reference to simulations: according to him a system property is emergent if it can be derived "only by simulation" (Bedau 2003, p. 15).

An alternative position on emergence has been advocated by Wimsatt (1986) even before computer simulations became widespread. Wimsatt (1986) starts out from analyzing the conditions for a system property to be a mere aggregate of the properties of the parts of which the system is composed (see also Wimsatt 2000, 2006a,b). Accordingly, a property of a system is called emergent if it does not satisfy these condition for aggregativity. In this way, Wimsatt is able to give a rather straightforward meaning to the dictum "a complex system is more than the sum of its parts" by relating emergence to the lack of aggregativity. What makes Wimsatt's position particularly interesting for this work is not only that relation between aggregation and emergence, but also the observation expressed by the following statements:

> [I]t is better to talk about properties of systems and their parts, and to analyze aggregativity as a kind of relation between these properties. (Wimsatt 1986, p. 260)

> Aggregativity and emergence concern the relationship between a property of a system under study and properties of its parts. (Wimsatt 2006a, p. 675)

The reason for which it is better to focus on properties, or rather to be explicit on that point, is that a system might be aggregative for one but emergent for another property. Just as a Markov chain might be lumpable with respect to one but non-lumpable with respect to another partition!

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