

Chapter 1

Overview: PCA models and issues

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Abstract Probabilistic cellular automata (PCA) are interacting discrete stochastic dynamical systems used as a modeling tool for a wide range of natural and societal phenomena. Their key features are: (i) a stochastic component that distinguishes them from the well known cellular automata (CA) algorithms, and (ii) an underlying parallelism that sets them apart from purely asynchronous simulation dynamics in statistical mechanics, such as interacting particle systems and Glauber dynamics. On the applied side, these features make PCA an attractive computational framework for high performance computing, distributed computing and simulation. Indeed, PCA have been put to good use as part of multiscale simulation frameworks for studying natural systems or large interconnected network structures. On the mathematical side, PCA have a rich mathematical theory that leads to a better understanding of the role of randomness and synchronicity in the evolution of large systems. This book is an attempt to present a wide panorama of the current status of PCA theory and applications. Contributions cover important issues and applications in probability, statistical mechanics, computer science, natural sciences and dynamical systems. This initial chapter is intended both as a guide and an introduction to the issues discussed in the book. The chapter starts with a general overview of PCA modeling, followed by a presentation of conspicuous applications in different contexts. It closes with a discussion of the links between approaches and perspectives for future developments.

1.1 Introduction

Cellular Automata (CA) are lattices of interconnected finite-state automata (also called cells) which evolve synchronously in discrete time steps according to deterministic rules involving the states of

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adjacent automata. That is, at each time-step each of the automata is updated independently of the others to a new value which is a function of the value of the automata in a suitably defined neighborhood. Their genesis is usually traced back to the 1948 paper by von Neumann and Ulam [174, 208] who introduced them as computational devices. An earlier, 1946 paper by Wiener and Rosenbluth [171] —modeling impulse conduction in cardiac systems— should also be considered a precursor. These papers already setup the scene for two important areas of application: *cybernetics* and *excitable media*. Interest in these systems was boosted in the 70s by Conway’s Game of Life —a two-dimensional cellular automaton— and in the 80s by Wolfram’s classification of one-dimensional automata.

CA are surprising computational tools whose dynamics, despite being defined through rather simple local rules, lead to a rich zoo of patterns and structures that emerge without being designed *a priori*. These structures can be transient, oscillating or stable, and can exhibit order at different levels of complexity or downright chaotic features. This richness has been exploited in a number of applications in different areas, of exact, natural and social sciences. They have even been proposed as an alternative discrete way to express physical laws using present computational tools [223, 211].

Probabilistic Cellular Automata (PCA) are the extension obtained when the rules for updating are allowed to be random: New values of each automaton are chosen according to probability distributions determined by the configuration of its neighborhood. Usually this updating is parallel or *synchronous* —all cells are simultaneously updated independently of each other— and neighborhoods are finite sets. At present, however, the notion of PCA is understood in a rather general sense, that includes (partially) asynchronous dynamics and not necessarily finite neighborhoods (see, *e.g.*, Chapter 16 and Chapter 18 below). In this book we adopt this general point of view.

The probabilistic component turns PCA into flexible computing tools for complex numerical constructions, and realistic simulation tools for phenomena driven by interactions among a large number of neighboring structures. PCA are, therefore, useful for the study of key issues of statistical mechanical and mathematical physics, such as phase transitions, metastability, percolation and transport theory. But they are also naturally adapted to the study of systems and processes in life and social sciences involving systems characterized by high levels of complexity and low level of reproducibility, even under extremely controlled conditions, due to inherent randomness or experimental limitations.

Mathematically, PCA are systems of Markov chains interconnected through a network which typically is a lattice or a finite sub-part of it. These Markov chains evolve in a parallel but coupled fashion, in which the distribution of future states of each chain depend on present states of neighboring chains. This coupling of transition probabilities is, however, local, and this makes PCA appealing as algorithms for high performance computing, distributed computing and simulations. Indeed, this locality makes the design of parallel implementations relatively straightforward, both on distributed architectures (*e.g.*, computing clusters) and on massively parallel architectures (*e.g.*, GPUs).

It is difficult to establish priorities and summarize the history of PCA developments. Their study was initiated by soviet mathematicians interested in artificial intelligence and cybernetics. Initially, PCA were studied to determine the robustness of CA dynamics subject to noise perturbation [203, 92]. In this setting, (non-)reliability is related to (non-)ergodicity [66]. The well-known North-East-Center PCA rule (see sub-section 1.3.1 below) was introduced in 1978 by Toom [204, for English translation] to provide a first PCA with a non-trivial instance of rigorously proven lack of ergodicity. Early applications also included models of neuronal networks [197], biological systems [206] and large systems of interacting automata [209]. In a somewhat independent way, PCA

were studied in the 70's and 80's by probabilists [53, 54, 89, 140, 141, 123] —interested in their properties as stochastic processes— and by statistical physicists [214, 112, 146, 104, 102] interested in the study of equilibrium and non-equilibrium statistical mechanical distributions on lattices. The interdisciplinary nature of PCA studies has led to a convoluted history of independent rediscoveries and alternative terminology. Initially, the automata were termed *locally interacting Markov chains*; other names include *stochastic CA* or *random CA*. Some references on applications are presented in Subsection 1.3.3. We refer to [185] and Part 1.4 in [159] for surveys on historical aspects.

This introductory chapter presents some general types of phenomena that have been represented through PCA, emphasizing open issues and challenges that will be discussed in the remainder of this book. Our goal here is to exhibit the main common ideas —that often traverse scientific boundaries—, leaving specific analyses for relevant chapters. In doing so we have preferred to follow our personal, hence subjective, viewpoints, avoiding exhaustiveness. We therefore apologize to the many important actors of the field whose work we have failed to cite.

The rest of this chapter is organized in four sections. They deal, respectively, with the following aspects: (1) Paradigmatic examples of PCA and their mathematical issues. (2) The three faces of the current interest in PCA: mathematical, computational and scientific modeling. (3) Useful links and future directions of research. (4) Summary of the structure of this book.

1.2 Phenomena addressed by PCA modeling

PCA dynamics belong to the category of *non-equilibrium lattice models*. In modeling circles, a *lattice* is a graph defined by a countable set of vertices (called sites or nodes) and a set of links. The latter are pairs of vertices usually visualized as a segment joining them. A popular lattice is, for instance, \mathbb{Z}^d . The cells or elementary components of the automata sit in the vertices and the links are interpreted as vehicles for interactions or communications between cells. Informally, the lattice is a network interconnecting the cells. The strength of an interaction between cells is expected to decrease with the number of mediating links (graph distance). Thus, the definition of the PCA usually involves a notion of *neighborhood* defined as vertices separated by a maximum prescribed number of links. In particular, two vertices are *nearest neighbors* if they are the endpoint of a link. The qualifier *non-equilibrium* refers to the type of questions addressed by the theory. To be sure, the issues of the existence, number, nature and basin of attraction of invariant (equilibrium) measures remain as important as in the theory of any stochastic process. Nevertheless, PCA theory focuses, particularly, in phenomena taking place *during the evolution* towards equilibrium. See for instance Chap 9 in this book.

In this section we describe three scenarios that lead to typical non-equilibrium issues addressed through PCA. The first one —metastability— refers to the appearance of traps and barriers delaying convergence. In some instances, these barriers are related to the emergence of non trivial collective behavior manifested as phase transitions. These statistical mechanics phenomena are also related to some highly challenging optimization issues [160, 1]. The second scenario (epidemiology) addresses the issue of survival vs extinction in large interacting populations. The third scenario (wildfires) illustrate the study of dynamic percolation phenomena. The mathematical treatment of the latter present some differences with the better known theory of equilibrium percolation models [110, 134, 212].

1.2.1 Metastability and traps

Phase transitions are one of nature’s more surprising phenomena. They refer to the sudden change on physical properties upon alterations of one or a few key parameters, for instance temperature or presence of a field: Liquids solidify at the freezing point, magnets acquire a non-zero magnetization even when the field is removed. In particular, *first-order phase transitions* are characterized by the presence of *coexistence curves*, that is manifolds of parameter values where the system presents several possible *stable phases*, *i.e.*, extremal equilibrium measures. Examples are water that at the right combinations of pressure and (low) temperature can be either in liquid or solid form, and magnets that at zero field and low enough temperature can be magnetized in different directions. In such conditions, the actual state of the system depends on how it is prepared: Water will remain solid if the coexistence curve is reached from the high pressure side and liquid if reached by increasing the pressure; the remaining magnetization of a magnet at low temperature will remember the direction the field had when turned off.

Phase transitions are equilibrium phenomena whose description involves no obvious reference to any dynamics. In contrast, the more mysterious phenomenon of *metastability* can only be understood through (stochastic) dynamical consideration. Physical systems exhibit metastable behavior in the vicinity of first order phase transitions, for instance in supercooled vapors and liquids, in supersaturated solutions and in ferromagnets undergoing *hysteresis*. The common feature is the persistence of the systems in a state that resembles one of the coexistent states in the transition curve, but is different from the true equilibrium associated to the actual value of the parameters: Supercooled water remains liquid at temperatures (slightly) below the freezing point; magnets during hysteresis point in a direction different from that of the (small) field present.

Typically, such state of affairs results from small temperature or field changes, performed in an extremely smooth fashion (by nature or by the lab technician). As a result the system finds that, in order to achieve the equilibrium corresponding to the new parameter values, it must overcome a “barrier” that is a remnant of the initial coexistence situation. The height of this “barrier” causes the system to remain for *extremely long times* in an apparent equilibrium —the *metastable state*— from which it will abruptly jump into the actual equilibrium as a result of some external perturbation or some internal random fluctuation. The observation of these metastability phenomena extends well beyond physics and includes processes in chemistry, biology, climatology, economics, *etc.*

A similar phenomenon takes place in numerical algorithms and simulation protocols whose convergence is often impaired by “traps” that retain the system for very long times. This type of metastability is of different nature than the one described above, as it is not due to a slight changes in parameters. Rather, the “traps” are an inherent feature of the dynamics, and the resulting evolution is closer to glassy transitions than to the neighbourhood of first-order ones.

All types of metastability manifestations share a number of attributes that point to the existence of a general theory. Such a theory should elucidate the following questions:

1. Distribution of the exit time from the metastable to the stable state. Typically this time is exponentially distributed with a rate that depends of the value of relevant parameters (temperature, magnetic field, type of “trap”).
2. Determination of the nature of the “metastable trap”. In gases and magnetic systems —and many asynchronous dynamics such as Metropolis or Glauber— the trap is associated to an “energy well”. This is far from universal, however; in some instances the trap is of purely entropic nature or, more generally, due to a “free-energy well”.

3. Details of the typical trajectories that the system takes when exiting the metastable state. This requires an understanding of the mechanisms behind this exit. In general, exit happens when a large atypical fluctuation allows the system to overcome the probabilistic barrier protecting the metastable situation. It is important to understand the nature of such a fluctuation. In many physical systems exit is due to *nucleation*, that is the emergence of a sufficiently large region looking as the stable state. In general processes, however, no such appealing mechanism seems to be available.

These three questions have been largely elucidated for many ferromagnetic systems — see [173, 23, 32] for finite-volume models (*i.e.* finite-size systems) and [190, 22] for models in infinite volume. Superheated water and supersaturated gas have been described through lattice-gas models subjected to Kawasaki dynamics — see [119, 100, 118, 172] in finite-volume and [119, 98, 99] for infinite volume. General overviews of these types of metastability phenomena are presented, for instance, in [176, Chapter 7] and [21].

Parallel dynamics open tantalizing perspectives for the understanding of metastability, because they exhibit metastable traps and exit mechanisms that differ from those of asynchronous dynamics and processes. In PCA these differences stem from the observation that *a large number of cells may change in a single time step*, leading to metastability mechanisms different from those of asynchronous dynamics. These facts make PCA metastability studies both a challenging [112, 61] and revealing component of the quest for a general theory of metastability. Comparative studies with asynchronous dynamics are particularly interesting, as they may lead to faster convergent simulation algorithms. See Chap. 3 in this book. For some pioneer studies on PCA metastability we refer to [40, 42, 45, 44, 41, 173]. A more general theory, that applies also to PCA, has been developed in [43].

1.2.2 Epidemics and extinction

A natural model in the epidemiology context is to consider a population of susceptible individuals sitting in the vertices of a lattice whose links determine the possibility of direct communication (interaction). The definition of the model includes:

- A set of possible states for each individual. Simple models assume three possibilities: sane/susceptible, ill/infected and recovered with or without immunity.
- A neighborhood of individuals that can pass the infection to a given one. Often, but not always, only nearest-neighbors are considered.
- A rule deciding when an infection is passed to an individual from his/hers neighbors.
- A rule specifying how one individual can recover and either become susceptible again or stay healthy forever due to acquired immunity.

The infection rule is stochastic in nature —exposition does not imply automatic contagion—, and so is the recovery rule. Furthermore, both rules should act on all individuals at the same time. PCA are, therefore, the model *par excellence* for epidemiological processes.

The rules depend on parameters that can be empirically estimated. For instance the probability that the individual at site k gets the infection at the n -th time-step can be of the form $1 - (1-p)^{N_k(n)}$, where $N_k(n)$ is the number of neighbors of k that are infected at time n . Here $p \in [0, 1]$ is a parameter that measures susceptibility to infection. The capacity to overcome the infection is, on the other

hand, an attribute of each individual. Hence, the probability of recovery of each individual at a given step is often assumed to be equal to another parameter $q \in [0, 1]$ independent of the rest of the population.

The main questions addressed to each epidemiology model refer to the range of parameters that will prevent the illness to become an epidemic. This is a risk management strategic question involving a number of measures: vaccines decrease p , isolation decrease N_k , general health situation increases q , *etc.* In relation to this, the order of magnitude of the *spreading time* is an important piece of information, as it determines optimal vaccination strategies or, if there is no time, the need for quarantine.

Whole families of *individual-based lattice models* have been introduced in the last decades. They are known by their acronyms, *e.g.* SIR (Susceptible, Infectious and Recovered), SIS (Susceptible, Infectious and Susceptible) (see for instance [19, 213, 188]). The propagation of computer viruses through technological networks is, of course, another natural area of application of epidemiological models [182]. This issue is also analyzed in Chap. 12 below.

1.2.3 Wildfire and percolation phenomena

Mathematical models can be an important aid in establishing policies to limit the damage caused by wildfires in forests. The model should answer, for a given spatial distribution of trees, questions such as “Will the whole tree population eventually burn?” or “What will be the shape of the front line of burning trees?” More generally the model should gauge the influence of the network structure and, hopefully, lead to the design of tree distributions for which the propagation to the whole forest is unlikely.

Wildfire models seem, conceptually, related to epidemiological models. Nevertheless, there is an important mathematical difference. Models in epidemiology deal with a finite population and focus on the persistence of the pathology *in time*. Wildfire models, on the other hand, consider a potentially infinite forest and study the *spatial* extension of the fire. The latter is, therefore, directly related to percolation models, as mentioned above. See [120] for recent related work as well as Chap. 5 and Chap. 14 in this book.

The mathematical ingredients of a wildfire model are the following. As usual, there is a lattice, for instance \mathbb{Z}^2 , with trees (potentially) sitting at its sites. The model is defined by the following choices.

- The possible states of each tree. In its simplest version it must include three possibilities: non-burning tree, burning tree and no tree (*e.g.* because it has burnt)
- Rule for the beginning of the fire. Possibilities are: the fire starts at a uniformly chosen tree (finite lattice), to simulate accidents, or ignition instances are (space-time) Poisson distributed to simulate lightning.
- Rule for the fire to pass from tree to tree. This should be a stochastic rule involving neighborhoods whose shape depends on actual conditions in the terrain. Examples include, but are not limited to, the nearest-neighbor CA. In general neighborhoods are assumed to be uniformly finite.

Let us, as example, detail the rules for the Drossel-Schwabl model. The situation at each site is represented by three possibilities: 0 (no tree), 1 (burning tree) and 2 (non-burning tree). All the

trees are simultaneously updated according to the following rules. Let us denote $\sigma_k(n)$ the state of the site k at time-step n .

- A burning tree disappears at the next time step:

$$\sigma_k(n) = 1 \mapsto \sigma_k(n+1) = 0 \quad \text{with probability } 1 .$$

- The growth of a new tree by chance at an empty node k is tuned through a parameter $p \in [0, 1]$

$$\sigma_k(n) = 0 \mapsto \sigma_k(n+1) = 2 \quad \text{with probability } p .$$

- A tree starts to burn at node k , either by ignition from another burning neighboring tree, or by chance. The later probability is given by a parameter f :

$$\sigma_k(n) = 2 \mapsto \sigma_k(n+1) = 1$$

with probability $\begin{cases} 1 & \text{if at least one neighboring tree is burning;} \\ f & \text{if no neighboring tree is burning.} \end{cases}$

Main general references on this specific model are [70, 69, 106]. An up-to-date reference for practitioners is [221]. Different critical behaviors have been studied in [107] through simulations and numerical analysis. Some theoretical results are given, for instance, in [48, 88]; see also [5].

1.3 The multiple faces of the PCA paradigm

CA and PCA were initially introduced both as theoretical models for *decentralized systems* and as computational tools. Eventually, however, they were seized by different scientific communities which exploited them in a number of directions, ranging from purely mathematical studies to practical modeling of natural structures. At present, PCA can be considered a code word for a “parallelization paradigm” that allows to clarify and deepen the understanding of fundamental issues in mathematics and physics while, at the same time, leading to efficient computational procedures and simulation algorithms. In Section 1.2 we discussed how the PCA paradigm contributes to the understanding of some key non-equilibrium phenomena. Here we focus, instead, on issues and features pertaining to the PCA dynamics in itself. These aspects are crucial for the design and trust of PCA as modeling and computational tools.

1.3.1 Mathematical issues

1.3.1.1 The mathematical setup

Unlike asynchronous dynamics —e.g. coupled differential equations, spin-flip dynamics or interacting particle systems— CA and PCA can be directly defined for infinite lattices of cells. Indeed, its parallel character ensures existence of the corresponding process without involving some finite-region limit or otherwise conditions on the parameters. We present in this section the main aspects

of the mathematical definition of the automata, starting with a list of the main ingredients of the setup:

The network G : This is a graph $G = (V(G), E(G))$ in which the set of vertices $V(G)$ marks the location of the automata (cells) and the set of edges $E(G)$ corresponds to interaction (or communication) channels between pairs of automata.

The alphabet S : Also called *local space* or *spin space*, describes the possible settings each automata may take. In most CA (for instance in this book) S is a finite set and hence it is endowed with the discrete σ -algebra and topology, and the uniform measure.

The configuration space $S^{V(G)}$: It represents the situation of the whole network of automata. It is endowed with the product topological and measure structure. Below we denote configurations as $\sigma = \{\sigma_k : k \in V(G)\}$, where σ_k is the configuration of the automaton at k .

The neighborhoods V_k : Each $V_k \subset V(G)$ represents the automata that can interact with the automaton sitting at $k \in V(G)$. For instance, a popular choice in $G = \mathbb{Z}^2$ is $V_k = \{k, k \pm e_1, k \pm e_2\}$ where (e_1, e_2) is the canonical basis of \mathbb{Z}^2 (north/south, east/west and center neighbors). This is the so-called *von Neumann* neighborhood.

CA are discrete-time dynamical systems

Deterministic cellular automata are defined by the iteration of a transformation (global update) of the form

$$F : S^{V(G)} \longrightarrow S^{V(G)}$$

$$(F(\sigma))_k = f_k(\sigma_{V_k})$$

for some single-updating functions $f_k : S^{V_k} \rightarrow S$. In many CA $V(G)$ admits the action of the group \mathbb{Z}^d . These actions are called *translations* and special emphasis is placed in translation-invariant CA, that is those whose updating rules commute with these translations.

As an illustration, let us consider the already mathematically rich CA in which $G = \mathbb{Z}$ (*one-dimensional PCA*). In this network translations are generated by the *shift* map

$$T : S^{\mathbb{Z}} \longrightarrow S^{\mathbb{Z}}$$

$$T(\sigma)_k = \sigma_{k+1}$$

Translation invariance amounts, then, to homogeneity of neighborhood's $V_k = V_0 + k$ and single-updating functions $f_k(\sigma) = f_0(T^{-k}\sigma)$ for some function $f : S^{V_0} \mapsto S$.

The Curtis-Hedlund-Lyndon theorem [115, Th. 3.1], characterizes translation-invariant CA transformations within the framework of dynamical systems. It states that a map F from $S^{\mathbb{Z}}$ to itself is a translation-invariant CA if and only if it is continuous (in the sense of the product topology) and commutes with the shift map. Moreover, if S has only two values, the map F is surjective if and only if it leaves invariant the uniform Bernoulli measure $\otimes_{k \in \mathbb{Z}} \mathcal{B}(1/2)$. We refer the reader to [155] for additional developments, to [130, 156] for recent results and to [142] for a recent survey of one-dimensional CA in the framework of topological dynamics. Readers interested in general introductions to CA are referred, for instance, to [129, 131]. See the Chap. 11 and Chap. 6 in this book.

PCA are interacting families of Markov stochastic processes

Stochastic updating rules are defined by Markovian transition-probability kernels. If $V(G)$ and the alphabet S are finite sets, these kernels are defined by functions of the form $P(\sigma | \eta)$, interpreted as the probability that a configuration η at time step t ($t \in \mathbb{N}$) will be updated into the configuration σ at time step $t + 1$. These functions must, therefore, satisfy the normalization condition

$$\sum_{\sigma} P(\sigma | \eta) = 1. \quad (1.1)$$

The Markovianness stems from the fact that the distribution of the new configuration σ is independent of preceding configurations other than immediately preceding η . In this finite setting, a PCA corresponds to transitions of the form

$$P(\sigma | \eta) = \prod_{k \in G} p_k(\sigma_k | \eta_{V_k}) \quad (1.2)$$

where $\{p_k(\cdot | \eta_{V_k}), k \in G, \eta_{V_k} \in S^{V_k}\}$ is a family of probabilities on S . The product (1.2) corresponds to a family of Markov processes, one at each site. Nevertheless, the processes interact with each other because they share a common past configuration η .

PCA, however, can be directly defined on infinite (but countable!) graphs G . In these CA, transition probabilities are defined by *probability kernels* on $S^{V(G)} \times S^{V(G)}$. These are functions $P(\cdot | \cdot)$ whose two arguments are of a different nature. Indeed, the kernel is a *probability measure* with respect to the first argument and a measurable function with respect to the second one. Explicitly, the requirements are:

- (i) $P(\cdot | \eta)$ is a probability measure on $S^{V(G)}$ for each $\eta \in S^{V(G)}$.
- (ii) $P(A | \cdot)$ is a measurable function for each measurable $A \subset S^{V(G)}$.

PCA stochastic dynamics correspond to kernels of the form

$$P(d\sigma | \eta) = \prod_{k \in G} p_k(d\sigma_k | \eta_{V_k}) \quad (1.3)$$

where each p_k is a probability kernel on $S \times S^{V_k}$. These product measures exist and are uniquely defined due to Kolmogorov existence theorem. CA correspond to the particular CA in which the measures $p_k(\cdot | \eta_{V_k})$ are *delta-like*.

It is important to distinguish PCA from interacting particle systems (IPS) [196, 149, 150, 62]. Both, PCA and IPS are Markovian processes defined by families of interacting stochastic processes. The difference lies in the level of (a)synchronism. IPSs update one spin per time step (or a few per unit time in the continuous-time version). Furthermore, the interactions in IPS models are not only due to a common past but also to constraints and penalties imposed at the arrival time. These aspects lead to delicate construction processes, involving limits of dynamics in finite parts of the graph, that may be feasible only under supplementary conditions on transition probabilities and rates. The study of processes on infinite graphs is not just mathematical entertaining, but it is made necessary by the huge number of entities composing real-life systems (10^{25} molecules in a cubic inch of fluid, 10^{11} neurons in the human brain).

Despite their differences, often PCA and IPSs offer alternative approaches to the study of the same type of phenomena. One instance is the transport mechanisms and phenomena studied through the *Totally Asymmetric Exclusion Process* that have similar manifestations in some PCA dynamics; see [139, 55, 147], [155, part 4.3] and Chapter 16 in this book.

The degree of synchronism also distinguishes PCA from Glauber-like spin-flip dynamics such as the ones used to simulate equilibrium spin models. PCA are specially suited for models in complete graphs, such as mean-field (e.g. Curie-Weiss) models, but can also provide efficient alternatives to study, with a controllable margin of error, the Ising and similar models [51, 143, 52, 179]. This issue is discussed in Chap. 7 below.

Let us also mention the results in [64, 162] where the cardinality of *directed animals* on the lattice is related to properties of some PCA dynamics. Exact solutions—that is, solutions determined by a closed system of a few analytic equations—have been found for some PCA. See, for instance, [127] for an exactly solvable non-reversible PCA.

1.3.1.2 Ergodicity and phase transitions

PCA in infinite graphs exhibit a rich taxonomy of invariant measures. These include product measures [156] and Markov random chains or fields [31, 49]. Further insight is achieved by studying space-time distributions [146, 151, 156] which, not surprisingly, are found to be related to statistical mechanical distributions in one further dimension [104, 146]. This relation is particularly fruitful for *reversible* PCA, that is for stochastic dynamics invariant under time reversal [137, 112, 61, 141, 151]. The connection between PCA and space-time statistical mechanics links the lack of ergodicity in the former with phase transitions in the latter. A PCA is *ergodic* if whichever its initial condition, it asymptotically converges in distribution to a unique invariant measure. In space-time picture, lack of ergodicity can often be related to a statistical mechanical phase transition triggered by boundary conditions on the initial space boundary of the space-time domain. Such lack of ergodicity was first rigorously exhibited in the simple (“toy”) models presented below. Let us point out that, for instance if all transition probabilities are strictly positive, the dynamics is ergodic for a finite number of automata but loses this property when the number of automata becomes infinite. This is a remarkable example of *global effect emerging* when infinitely-many sites interact.

Phase transitions are associated to multiple invariant measures. It is natural to wonder whether when the invariant measure is unique the automata is necessarily ergodic (that is, this measure is attained for all initial configurations). The answer is negative [36, 125]. Transition probabilities usually depend on one or several parameters. The catalog of invariant measures for different values of those is called a *phase diagram*, in analogy with the statistical mechanical nomenclature. The rigorous determination of phase diagrams is often a difficult task and numerical studies are the only available option. See [195] for a numerical analysis of the phase diagram of some *majority voter* PCA. See also Chap. 15 below.

The Stavskaja model

This is the first model in which lack of ergodicity was rigorously proven. The model, to be considered in Chap. 13, depends on a *noise* parameter $\varepsilon > 0$. Its definition is as follows:

(S1) Graph $G = \mathbb{Z}$.

- (S2) Alphabet $S = \{0, 1\}$.
 (S3) Neighborhoods $V_k = \{k-1, k\}$.
 (S4) Updating rule: For $\varepsilon \in [0, 1]$ fixed

$$p_k(1 \mid \eta_{\{k-1, k\}}) = \begin{cases} 1 & \text{if } \eta_k = \eta_{k-1} = 1 \\ \varepsilon & \text{otherwise} . \end{cases} \quad (1.4)$$

For $\varepsilon = 0$, this is the elementary CA with rule 192 (Wolfram’s denomination [214]) —see Table 1.1. Such rule is not symmetric under the interchange $0 \leftrightarrow 1$ but has both configurations $\underline{1}$ (“all ones”) and $\underline{0}$ (“all 0”) as fixed points. If $0 < \varepsilon < 1$ the dynamics can be thought as Rule 192 followed by a

V_k ’s pattern at time $n-1$	111	110	101	100	011	010	001	000
new state in k at time n	1	1	0	0	0	0	0	0

Table 1.1 Elementary Cellular Automata rule 192.

non-symmetric noise —*error mechanism*— which flips “0” into “1” independently with probability ε while leaving “1” unaltered. The resulting PCA has the following properties:

- (SN1) The configuration $\underline{1}$ is absorbing, already in finite volume.
 (SN2) The rates are not all (strictly) positive.
 (SN3) The dynamics is not reversible.

The Stavskaja PCA is ergodic in its finite-graph version, but the ergodicity is lost for the full lattice for small values of ε . The precise result is as follows.

Theorem 1. *For the PCA defined by (S1)–(S4) above there exists a critical value $\varepsilon^* > 0$ such that:*

- (i) *If $\varepsilon > \varepsilon^*$ the dynamics is ergodic with $\lim_{n \rightarrow \infty} \mathbb{P}_\rho(\sigma(n) = \cdot) = \delta_{\underline{1}}(\cdot)$ for any initial distribution ρ .*
 (ii) *If $0 < \varepsilon < \varepsilon^*$ there is a second invariant measure in which the value 0 survives:*

$$\lim_{n \rightarrow \infty} \mathbb{P}_{\delta_{\underline{0}}}(\sigma(n) = \cdot) = \mu_\varepsilon(\cdot) \neq \delta_{\underline{1}} . \quad (1.5)$$

Furthermore, every translation-invariant stationary distribution is a convex combination of μ_ε and $\delta_{\underline{1}}$.

The proof was first described in [191] and spelled out in [210]. More recent developments are given in [164, 59, 200] and Chap. 13. The exact value ε^* is still unknown. Numerical simulations and estimation give $\varepsilon^* \sim 0.29450$. Figure 1.1 shows a sample of a space-time diagram for ε slightly subcritical.

The North-East-Centre PCA model and the erosion property

This very celebrated PCA is defined as follows:

- (N1) Graph $G = \mathbb{Z}^2$.
 (N2) Alphabet $S = \{0, 1\}$.

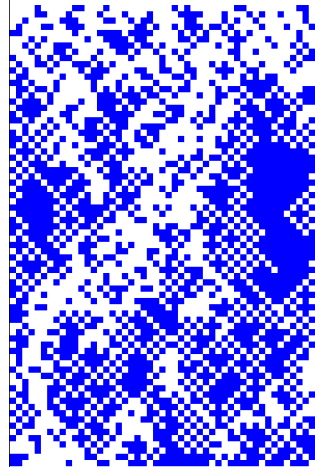


Fig. 1.1 Sample of a space-time configuration of the Stavskaja model. The parameter value is $\varepsilon = 0.28$. Boundary conditions were chosen periodic. The initial configuration is a central activated site (1) and the other sites are inactivated (0). Black (resp. white) squares represent activated (resp. inactivated) sites. Time is running downwards. Simulated using FiatLux software [77].

(N3) Neighborhoods $V_k := \{k, k - e_1, k + e_2\}$.

(N4) Updating rule: For $\varepsilon \in [0, 1]$ fixed

$$p_k(0 \mid \eta_{V_k}) = (1 - \varepsilon)(1 - \text{Maj}(\eta_{V_k})) \quad (1.6)$$

where $\text{Maj}(\sigma_x, \sigma_y, \sigma_z)$ is the value adopted by the majority of the three arguments.

For $\varepsilon \in]0, 1[$, the NEC PCA is a noisy perturbation of the *majority* CA, defined by

$$f_k(\sigma_{V_k}) = \text{Maj}(\sigma_{V_k}) . \quad (1.7)$$

The error mechanism is, in fact, identical to that of the Stavskaja PCA and, as a consequence, the NEC shares with the latter the features (SN1)–(SN2) listed above. The NEC PCA, however, has many more absorbing configurations, for instance those formed by an arbitrary number of vertical and/or horizontal lines filled with “1”.

The NEC PCA has, however, two additional properties that act in opposed direction and which are responsible for very eventful space-time diagrams:

The erosion property: The associated CA (1.7) is such that finite sets of “1” sites in an otherwise all “0” configuration disappear in a finite time, and similarly for islands of “0” inside a “1” sea.

Alignment-suppression property: There exist “spiders” formed by a few segments of sites such that, once they are filled with “1”, the dynamics propagates these “1” to the interior of a sphere. As discussed in [84] this means that presence of a sphere of “1” is penalized by the invariant measures only as a sub-volume exponential. This contradicts well known Gibbsian properties and implies that *all* invariant measures for the NEC are *non-Gibbsian*.

The loss of ergodicity for small ε was proven by Toom [203] introducing carefully defined space-time contours and has since become a model argument to prove non-ergodicity in PCA. There has been a number of rewriting, reinterpretation, refining and extensions of this pioneer proof. Interested readers can consult, for instance, Chap. 13 and [153, 178, 15, 65, 111].

The Positive Rate Conjecture

There exist different sets of sufficient conditions ensuring ergodicity of PCA [154, 85, 152, 46]. Many of those require local updating with *positive rates*:

$$p_k(s \mid \eta_{V_k}) > 0, \quad \forall k \in G, s \in S, \eta_{V_k} \in S^{V_k}. \quad (1.8)$$

This property implies that all pair of configurations have positive probabilities of being mutually reachable. In particular no absorbing states are possible. The long standing *positive-rates conjecture* stated that all positive-rate PCA on $G = \mathbb{Z}$ are ergodic. This conjecture was proved to be false through a complicated example in [93, 108]. The design of an understandable counterexample with $S = \{0, 1\}$ is still an open problem.

1.3.1.3 Random perturbations of CA

One of the motivations of introducing PCA was to study the stability of CA under random perturbations. In this regard, the non-ergodicity results of the Stavskaja and NEC PCA reported above point in the direction of stability of the Rule 192 (Table 1.1) and majority [rates (1.7)] CA under an asymmetric noise that flips “0” into “1” with probability ε . Indeed, the perturbation is proven to preserve both CA fixed points $-\delta_{\underline{1}}$ and $\delta_{\underline{0}}$ — though the latter becomes a non-trivial probability measure supported in configurations that include infinitely many “1” (due to the erosion property). The question arises as to how dense these “1” are.

Kinzel [136] studied this question for stochastic perturbations of the CA defined by rule 90 in Wolfram’s denomination [214] (Table 1.2). Performing a non-rigorous extrapolation from finite-size

V_k ’s pattern at time $n - 1$	111	110	101	100	011	010	001	000
new state in k at time n	0	1	0	1	1	0	1	0

Table 1.2 Elementary Cellular Automata rule 90.

scaling, Kinzel concluded that the invariant measure obtained by perturbing $\delta_{\underline{0}}$ has zero density of “1” for small noise. This conclusion was shown to be false in [24], for arbitrarily small asymmetric noise. As soon as $\varepsilon > 0$, the probability of survival of “1” is strictly positive uniformly in the size of the system. This shows that even a very small noise can change properties drastically and, incidentally, that to formalize arguments based on finite-size scaling is a delicate task.

The proof in [24] is based on a connection with a process of *oriented percolation*. This type of connections has been later exploited, for instance, in [67]. The connection of PCA long-time behavior with processes of directed percolation is part of the epidemiology scenario discussed above and has been developed in [71, 132, 181, 165, 175, 133].

1.3.2 Computational issues

Synchronous, or quasi-synchronous updating turn PCA into natural tools for efficient parallel computing algorithms [56, 57, 217]. Here we present the main issues addressed by the theory of CA and PCA as computational tools.

CA as universal computational systems

A computational system is said *universal* if it can run any program or, equivalently, execute any algorithm. Such attribute can be exhibited, for instance, by proving that the system can run programs equivalent to any program run by a Turing machine. The first CA proven to be computationally universal was Rule 110 (Table 1.3), analyzed in [47]. Recently, there have been exhaustive studies [198, 161] on the computational properties of all the elementary cellular automata (ECA) in Wolfram’s classification [214].

V_k 's pattern at time $n - 1$	111 110 101 100 011 010 001 000
new state in k at time n	0 1 1 0 1 1 1 0

Table 1.3 Transition’s rules of elementary Cellular Automata rule 110.

CA and PCA as decentralized computational systems

Both CA and PCA are archetypical models of *decentralized computing*. Each cell has its own resources and operates at each time step exchanging information and results only with neighboring units. Global features of the system emerge as collective results of these local interactions, without being driven by any external rule (or only partially ruled by external factors, as could be argued for global magnetic fields in Ising-like systems). The attributes of the computational approach offered by cellular automata are appropriately summarized in the “formula” stated in [193]:

simple + parallel + local = cellular computing .

Outputs of CA and PCA provide instances of self-organizing behavior, and constitute a natural framework to relate this with the theory of formal languages and measures of algorithmic complexity. These issues are discussed in [216]. See also [34] for an introduction to algorithmic complexity.

PCA as stochastic algorithms

Stochastic algorithms tend to have better convergence properties than deterministic ones. Perhaps the main reason is that the former incorporate mechanisms to avoid or escape the drift towards local minima that constitute terminal traps for the latter. Nevertheless, in the presence of randomness these traps become metastable states from which escape times, though always finite, can become

excruciatingly long. At this point the mathematical issue of ergodicity, discussed above, has a direct relevance.

In finite networks, most PCA dynamics can be proven to be ergodic, guaranteeing the eventual convergence of the associated algorithm to a well defined final law. This is a consequence of general results in the theory of Markov chains, which apply for instance to positive rates PCA dynamics. Nevertheless, finite systems are expected to exhibit metastable behavior if the associated infinite system undergoes a phase transition/loss of ergodicity phenomenon. This is a well-known fact for MCMC practitioners [74, 128]. The issue was rigorously studied for a parallel implementation of the Gibbs sampler associated to the Ising Hamiltonian [112, 61, 40, 49] and in connection with the simulated annealing approach for stochastic algorithms [86].

PCA and robustness with respect to errors

PCA constitute, on the one hand, the natural framework to study sensitivity to round off and other sources of errors in CA computations and, on the other hand, an excellent laboratory for the design of robust and trustworthy computational approaches. This perspective has been analyzed in [92, 111] and, more recently, in [183, 83, 16].

Ergodicity, in particular, corresponds to (extreme) robustness with respect to the initial conditions. The ergodicity for a PCA dynamics on $G = \mathbb{Z}$ is proven to be undecidable from an algorithmic point of view. See [205, 28] and [155, subsection 3.1]. In a complementary way, the sensitivity to starting conditions implied by the absence of ergodicity has also been put to good use through PCA computations. A conspicuous example are the PCA dynamics that solve the *majority* or *density-classification* problem, namely to determine, on the basis of large-time outputs, whether there was a majority of some spin value in the starting condition [90, 163, 80, 4]; see Chap. 10 below.

Synchronicity and updating schemes

While parallel (synchronous) updating has obvious mathematical and computational advantages, sequential (asynchronous) updating has also important favorable features. For instance, the latter is well adapted to simulations of short-range spin models and, on the practical front, does not require the existence of a universal clock to which all the automata must synchronize. Furthermore sequential sampling can be fine-tuned by adopting an appropriate updating scheme (e.g. uniformly at random, random with respect to the last updated node or deterministic).

The question arises whether efficiency can ultimately be improved by adjusting *both* the degree of synchronicity and the updating scheme. This issue has been actively investigated in the last two decades [18, 2, 184, 35, 82, 58]. A promising alternative are the so-called α -asynchronous PCA in which, when updating time arrives, the node is updated with probability α and otherwise left invariant. See the survey paper [79] and the references therein for more details.

1.3.3 Applications of PCA

PCA models have found applications in a diversity of fields from exact, natural and social sciences. We offer in this section an overview of the reach of these applications.

PCA as a flexible modeling and simulation framework in a variety of applied contexts

The seminal work of Vichniac [211] placed CA as an *exact* modeling alternative to differential equations and not only as an approximation scheme [201, 159]. See for instance [124] for a comprehensive development. Here is a comparative list of advantages of cellular automata approaches:

- PCA models are simple to define if rules are given on a context-dependent basis. They provide a complete description of the evolution of the system even at the level of individual agents (cells) or of clusters of few individuals (“low-level” description).
- Models based on differential equations are suitable, in general, only for large space and time scales and if there is some level of homogeneity or some “steering global influence” that justifies a description in terms of densities.
- PCA belong to so-called *individual-based models*, that is:
 - They are based on information given at the individual level and, therefore, have a number of variables proportional to the number of individual cells.
 - Simple low-level rules are the only source of the complex global phenomena or *collective behavior* that may eventually emerge at the level of the whole population or of a high fraction of its individuals (“high-level” phenomena).
- Unlike differential equations, PCA can incorporate specific individual attributes. The framework is particularly appropriated for systems which can be decomposed into interconnected elementary entities and where there is lack of homogeneity like in biological systems.
- PCA approaches can describe fluctuations which integro-differential approaches in general smooth out, average or neglect.
- PCA modeling applies at scales where no averaging is reasonable and therefore not amenable to analysis through differential equations.

Some general references on the connection between low- and high-level scales are [192, 60, 177], and [12, 187] for modeling considerations. Of particular interest is the recent development of *hybrid models* involving different time or space scales. We cite for instance [167] where a CA approach is used with an environment governed by a partial differential equation. Another original contribution is the reverse engineering approach developed in [122] to find out PCA rules able to generate some fixed experimental patterns.

As a preliminary glimpse for interested readers here is a (very incomplete!) overview of modeling applications of PCA in different scientific and technological areas.

PCA as models for complex systems

PCA dynamics have two distinctive features:

- *Emergence*: Complex collective behavior appears solely as a result of local rules. We refer to [145, 109] for a general presentation of the *emergence* concept in physics, life sciences and economical and other social phenomena.
- *Multiscale behavior*: This emergence acts at different scales with different levels of complexity. This multiscale feature is, in fact, a trademark of complex phenomena. See, for instance, [158] and the recent book [116] for a discussion of this aspect of the automata.

These attributes make PCA one of the most used class of models to analyze complex systems [215, 38, 13, 11]. PCA simulations are useful to understand complex behavior and to make predictive analysis. These predictions can often be rather surprising and counter-intuitive, as illustrated in Chap. 18 of this book.

PCA as models for life sciences

PCA systems are of great value in biological modeling, due to their sensitivity to space heterogeneity and their capacity to give rise to self-organized global structures. See [95] for a survey of life science applications and [116, 166, 10] for general modeling considerations. More specifically, PCA have been successful tools to describe pattern formation in cell development (*morphogenesis*) [63, 206] and cell biology [39, 96], specially in relation to multiscale phenomena [189, 3, 114, 60]. Other applications include immunology [202, 219, 26, 222]; neurosciences [105, 138, 135, 157, 94] and Chap. 17 of this book; oncology [126, 60, 199], and epidemiology [148, 19, 91, 168, 194, 213, 75].

In ecology, PCA models have long being proposed both as a paradigm [117] and to describe or simulate concrete issues. These include, for instance, evolution [180] and population dynamics [87, 29]. Most of the studies were of numerical character, but some rigorous results are also available [73, 169]

To conclude, let us mention, as part of the life sciences applications, a stochastic extension of the famous *game of life* (deterministic) CA, which was studied through computer simulations [170].

PCA as models for social sciences

Opinion dynamics have been modeled through PCA in which spin values correspond to voting opinions [8]. The use of PCA systems has been advocated [14, 76] to model the evolution of markets driven by economic or financial agents. Such models have been applied to study *crisis propagation* in a network of companies, discriminating among different regimes that range from almost independent entities to strongly interconnected markets [14, 121, 103, 50]. See Chap. 4 below.

PCA as models for exact sciences

PCA have been proposed as a general model for physical phenomena [37]. At present, the literature involving PCA in physics and chemistry is immense. Readers can consult the proceedings of the 2014 International Conference on Cellular Automata for Research and Industry [113] to have an idea of the state of the art. Recent notorious contributions range from an analogy with chemical reactions [186] and traffic models [220]. See also Chap. 16 of this book for a study of transport in lattice gases.

PCA as models for art

Perhaps not surprisingly given the plethora of patterns cellular automata can produce, PCA have also found applications in the visual arts. See [81] and Chap. 1.5 of this book.

1.4 Future perspectives

As a result of the intense activity in PCA modeling, both theory and applications are moving into new directions that require extensions and refinement of the present conceptual framework and available techniques. Here are some pressing issues.

General alphabets

All the automata studied so far have finite discrete alphabets. The need to consider more general alphabets—including, perhaps, some global constraints—relies both on mathematical [30] and modeling reasons (see e.g. Chapters 18 and 19 of this book). Here are further examples that justify the development of a more general theory:

- Cellular Potts models for biological tissues require very large alphabets.
- The swarming model considered in Chap. 16 is a fully synchronous PCA with some conserved quantities.
- Countable spin spaces are considered in an ecological context in [17].
- In Chap. 8, the interacting Pólya urn model is seen as a PCA with $S = [0, 1]$. Automata with continuous alphabets are sometimes called *continuous automata* [33].

General interactions

Historically, the interactions among automata have been of finite range. This is consistent with the interest in computer science to settle questions relating local and global transfer of information. Nevertheless, the modeling of dynamics of complex systems or the simulation of non-equilibrium statistical mechanical systems require more general types of interactions. A few examples:

- Models with global constraints [78], Chapters 16, 18 in this book and [7] (swarming models; silicon cells as in the CPM model, and models for glioma cell migration).
- Mean-field interactions, modeled in versions used for equilibrium spin models [25, 9, 144].
- Theoretical generalizations of PCA for simulation purposes [6].

Disorder

The architecture and the parameters of real-life networks are themselves subject to errors and fluctuations. Appropriate models require, then, the introduction of disorder either in interaction parameters—like in random field Ising models [20]—or in the underlying graph where the automata

sits —like the power-law random graphs describing social and electronic networks [68, 218]. Yet another type of disorder of interest is the one characterizing the *stochastic spatial models* [72], in which sites can “mutate” their state. Updating rules can also change in a disorderly fashion. This possibility can be related to the issue of using observed data to statistically infer updating rules as in Chap. 20 of this book.

Implementation as computational schemes

The exceptional potential of PCA for high performance computations has not yet been fully exploited for research-oriented simulations and computations. Some pioneer examples that point the way for future developments are the following.

- The implementation [143] (and Chap. 7) of a toy PCA on parallel architectures (like GPU units) for theoretical research purposes.
- The implementation on parallel architecture of classical stochastic algorithms (MCMC, Gibbs sampling, stochastic approximation). It can be done in a synchronous or quasi-synchronous way [97].
- The use of PCA in [101] to find large cliques in Erdős random graphs.
- The connection to statistics and machine learning algorithms recently presented in [207].

1.5 Structure of the book

PCA have deservedly gained widespread recognition as versatile and efficient computational and simulation tools. They are presently been used in many areas of knowledge ranging from pure probability to social studies and including a wealth of scientific and technological applications. Furthermore, they constitute interesting mathematical objects on their own, whose theory lies at the crossroad of probability, statistical mechanics and theoretical computer science. This situation has led to a highly diversified pool of theoreticians, developers and practitioners whose interaction is highly desirable but can be hampered by differences in jargon and focus.

This book —as the workshop in which it is based— is an attempt to approach these different research communities by offering a tribune for them to present achievements, pressing issues and future directions. The book is not intended as a treatise, but rather as a gentle introduction, for a general readership, of the role and relevance of PCA technology. The goal is to foster interest of newcomers and interaction between the different community-dependent perspectives, hopefully promoting new syntheses and applications. Each chapter can be read independently, in particular it carries its own bibliography section. Notation and formal aspects vary, according to standard usage in each research area, but differences are not dramatic and transitions should be straightforward for the reader.

The remaining of the book is divided in three parts oriented towards different families of applications:

Part I: Probability and statistical mechanics. Its seven chapters deal with probabilistic issues arising from the use of PCA as statistical mechanical models. These models share properties—and have

contrasting attributes— with the standard sequential stochastic models used in out-of-equilibrium statistical mechanics.

Part II: Computer science and discrete dynamical systems. The six chapters of this part are devoted to central questions regarding robustness and computational aspects of PCA. Issues include comparisons with deterministic CA, general mathematical properties (e.g., convergence to a fixed point, phase transitions, existence of invariant measures) and determination of computations best suited to the use of PCA (e.g., density classification [27, 80]). Here, the term “computation” is intended in a general sense which includes, for instance, pattern formation [63] and classification of initial conditions. A particularly interesting question is to which extent randomness helps to speed up computations.

Part III: Applications to natural sciences and computational (cell) biology. It is formed by five chapters with applications to cell functions (e.g. Cellular Potts Model and stability of emerging patterns), challenging aspects of computational biology (Chap. 17, Chap. 18 and Chap. 19) in particular weakened parallel with CPM, and multiscale modeling of atmospheric or oceanic circulation (Chap. 20). Chap. 16 introduces a model of swarming.

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