Construction of local structure maps for cellular automata

Henryk Fukś

Department of Mathematics
Brock University
St. Catharines, Ontario L2S 3A1,
Canada
Email: hfuks@brocku.ca

Abstract

The paper formalizes and extends the idea of local structure approximation for cellular automata originally proposed by Gutowitz et. al. [1]. We start with a review of the construction of a probability measure on the set of bi-infinite strings over a finite alphabet of \( N \) symbols. We then demonstrate that for a shift-invariant probability measure, probabilities of all blocks of length up to \( k \) can be expressed by \((N - 1)N^{k-1}\) linearly independent block probabilities. Two choices of these independent blocks are discussed in detail, one in which we choose the longest possible blocks (“long form”) and one in which we choose the shortest possible blocks (“short form”). We then proceed to review the method which allows to approximate probabilities of blocks longer than \( k \) by blocks of length \( k \) or less. This approximation, known as Bayesian extension or Markov measure, is then used to construct approximate orbits of shift-invariant probability measures under the action of probabilistic or deterministic cellular automaton. We show that the aforementioned approximate orbit is completely determined by an \((N-1)N^{k-1}\)-dimensional map. When the short form of block probabilities is used, this map takes particularly simple form, often revealing important features of a particular cellular automaton.

1. Introduction

Cellular automata (CA) are often considered as maps in the space of Borel shift-invariant probability measures equipped with the weak\(^*\) topology [2 3 4 5]. The central problem of the theory of cellular automata in this setting is to determine properties of orbits of given initial measures \( \mu \) under the action of a given cellular automaton. Since computing the orbit of a measure is in general very difficult, approximate methods have been considered. The simplest of these methods is called the mean-field theory, and has its origins in statistical
The main idea behind the mean-field theory is to approximate the consecutive iterations of the initial measure by Bernoulli measures. While this approximation is obviously very crude, it is sometimes quite useful in applications.

In 1987, H. A. Gutowitz, J. D. Victor, and B. W. Knight proposed a generalization of the mean-field theory for cellular automata which, unlike mean-field theory, takes (partially) into account correlations between sites. The basic idea of local structure theory is to consider probabilities of blocks of length $k$ and to construct a map on these block probabilities, which, when iterated, approximates probabilities of occurrence of the same blocks in the actual orbit of a given cellular automaton. The construction was based on the idea of “Bayesian extension”, introduced earlier by other authors in the context of lattice gases, and also known as a “finite-block measure” or as “Markov process with memory”.

In the original paper, Gutowitz et. al. made a compelling argument that “the local structure theory appears to be a powerful method for characterization and classification of cellular automata”. After performing extensive Monte-Carlo simulations and statistical analysis they concluded that the local structure “is an accurate model of several aspects of cellular automaton evolution. The dependence on initial conditions and convergence properties are well modeled by the theory. It appears that, even for complex rules, the stable invariant measures of a cellular automaton may be estimated to arbitrary resolution”.

In the last 25 years, the local structure theory has been applied to study various aspects of dynamics of both deterministic and probabilistic cellular automata, including, for example, such topics as classification of CA, phase transitions in probabilistic CA, CA models of traffic flow, asynchronous CA, and many others. In spite of this, there has been virtually no effort to study this theory from a more formal point of view, in order to obtain rigorous results which could be confronted with Monte Carlo experiments and numerical simulations. This paper is intended to be a first step toward filling this gap.

The paper is organized as follows. In the first section, we review the classic construction of measures on $\mathcal{A}^\mathbb{Z}$, where $\mathcal{A} = \{0, 1, \ldots, N - 1\}$, using cylinder sets and the Hahn-Kolmogorov extension theorem. In the next section we show that for a shift-invariant measure, measures of all cylinders sets of length up to $k$, which we call “block probabilities”, can be generated by $(N - 1)N^k$ linearly independent block probabilities. We describe two choices of these independent blocks probabilities, “long form” and “short form”. In section 4 we show how the knowledge of measures of cylinder sets of length up to $k$ can be used to approximate the entire measure. This construction is sometimes known as the “maximal entropy” extension. We present proof of the maximality of the entropy following the idea given in [9] and adopted to our formalism.

The maximal entropy extension is then used to construct approximate orbit of a measure $\mu$ under the action of cellular automaton. Points of this orbit are entirely determined by $(N - 1)N^k$ block probabilities, thus it is possible to generate approximate orbits by iterating $(N - 1)N^k$-dimensional real maps, instead of much more complicated $N^k$ dimensional maps proposed in [1]. We also show that, as $k$ increases, every point of the approximate orbit weakly converges to the corresponding point of the exact orbit.

Finally, we present some examples of local structure maps and their reduced form.
2. Construction of a probability measure

Let \( \mathcal{A} = \{0, 1, \ldots, N - 1\} \) be called an alphabet, or a symbol set, and let \( X = \mathcal{A}^\mathbb{Z} \). The Cantor metric on \( X \) is defined as \( d(x, y) = 2^{-k} \), where \( k = \min\{|i| : x_i \neq y_i\} \). \( X \) with the metric \( d \) is a Cantor space, that is, compact, totally disconnected and perfect metric space. A finite sequence of elements of \( \mathcal{A} \), \( b = b_1b_2\ldots b_n \) will be called a block (or word) of length \( n \). Set of all blocks of elements of \( \mathcal{A} \) of all possible lengths will be denoted by \( \mathcal{A}^* \).

Elementary cylinder set generated by the block \( b = b_1b_2\ldots b_n \) and anchored at \( i \) is defined as

\[
|b|_i = \{x \in \mathcal{A}^\mathbb{Z} : x_{i,i+n} = b\},
\]

where we require that one of the indices \( i, i+1, \ldots, i+n-1 \) is equal to zero, or, equivalently, that \( -n+1 \leq i \leq 0 \). For a given elementary cylinder set \( |b|_i \), indices \( i, i+1, \ldots, i+n-1 \) will be called fixed, while all other indices will be called free. The requirement \( -n+1 \leq i \leq 0 \), therefore, means that the origin is always fixed. The collection (class) of all elementary cylinder sets of \( X \) together with the empty set and the whole space \( X \) will be denoted by \( \text{Cyl}(X) \). We will use the convention that for \( b = \emptyset \), \( |b|_i = X \).

Let \( |a|_j \) and \( |b|_i \) be two elementary cylinder sets. We will say that \( p \in \mathbb{Z} \) is a matching (mismatching) index of these cylinder sets if for every \( x \in |a|_j \), \( y \in |b|_i \) we have \( x_p = y_p \) \( (x_p \neq y_p) \). An index which is either matching or mismatching will be called overlapping index. Note that since we require that the origin is fixed, any two cylinder sets must have at least one overlapping index.

**Proposition 2.1** The collection of all elementary cylinder sets together with the empty set and the whole space constitutes a semialgebra over \( X \).

**Proof:** In order to show that elementary cylinder sets constitute a semialgebra we need to prove (i) the closure under the intersection and (ii) that the set difference of two elementary cylinder sets is a finite union of elementary cylinder sets.

For (i), let \( |a|_j \) and \( |b|_i \) be two elementary cylinder sets. As such, they must have some overlapping indices. If all overlapping indices are matching, then \( |a|_j \cap |b|_i \) is just the elementary cylinder set generated by overlapped concatenation of \( a \) and \( b \). If among overlapping indices there is at least one mismatching index, then \( |a|_j \cap |b|_i \) is empty.

For (ii), let us observe that

\[
X \setminus |b|_i = \bigcup_{j=0}^{n-1} \{x \in X : x_{i+j} \neq b_{j+1}\}. \tag{2}
\]

Each of the sets \( \{x \in X : x_{i+j} \neq b_{j+1}\} \) can be expressed as a union of elementary cylinder sets, thus \( X \setminus |b|_i \) is also a union of elementary cylinder sets. Now, since

\[
|a|_j \setminus |b|_i = |a|_j \cap (X \setminus |b|_i), \tag{3}
\]

and (i) holds, we obtain the desired result. \( \square \)

\footnote{Other choices of elementary cylinder sets are possible, not requiring fixed origin — see, for example, \[5\]. Our choice is motivated by the desire that the set of elementary cylinder sets is closed under intersection.}
We will now introduce the notion of a measure on the semi-algebra of cylinder sets. Let \( \mathcal{D} \) be a semialgebra. A map \( \mu : \mathcal{D} \rightarrow [0, \infty] \) is called a measure on \( \mathcal{D} \) if it is countably additive and \( \mu(\emptyset) = 0 \). By countable additivity we mean that for any sequence \( \{A_i\}_{i=1}^{\infty} \) of pairwise disjoint sets belonging to \( \mathcal{D} \) such that \( \bigcup_{i=1}^{\infty} A_i \in \mathcal{D} \),

\[
\mu \left( \bigcup_{i=1}^{\infty} A_i \right) = \sum_{i=1}^{\infty} \mu(A_i). \tag{4}
\]

For measures on the semialgebra of cylinder sets, countable additivity is implied by finite additivity.

**Proposition 2.2** Any finitely additive map \( \mu : \text{Cyl}(X) \rightarrow [0, \infty] \) for which \( \mu(\emptyset) = 0 \) is a measure on the semialgebra of elementary cylinder sets \( \text{Cyl}(X) \).

**Proof:** We start with a remark that in the Cantor topology elementary cylinder sets are clopen, that is, both closed and open.

Suppose now that the map \( \mu \) satisfies \( \mu(\emptyset) = 0 \) and is finitely additive, that is, for any finite sequence \( \{A_i\}_{i=1}^{m} \) of pairwise disjoint sets belonging to \( \text{Cyl}(X) \) such that \( \bigcup_{i=1}^{m} A_i \in \text{Cyl}(X) \),

\[
\mu \left( \bigcup_{i=1}^{m} A_i \right) = \sum_{i=1}^{m} \mu(A_i). \tag{5}
\]

In order to show that \( \mu \) is a measure on \( \text{Cyl}(X) \), we need to show that it is countably additive. Let \( B \) be a cylinder set and let \( \{A_i\}_{i=1}^{\infty} \) be a collection of pairwise disjoint cylinder sets such that \( \bigcup_{i=1}^{\infty} A_i = B \). Since \( B \) is closed, it is also compact. Sets \( A_i \) are open, and form a cover of the compact set \( B \). There must exist, therefore, a finite subcover, that is, a finite number of sets \( A_i \) covering \( B \). Moreover, since \( A_i \) are mutually disjoint, there must exist \( m \) such that \( A_i = \emptyset \) for all \( i > m \), and therefore \( B = \bigcup_{i=1}^{m} A_i \). Then by finite additivity of \( \mu \) and the assumption that \( \mu(\emptyset) = 0 \) we obtain

\[
\mu(B) = \mu \left( \bigcup_{i=1}^{\infty} A_i \right) = \mu \left( \bigcup_{i=1}^{m} A_i \right) = \sum_{i=1}^{m} \mu(A_i) = \sum_{i=1}^{\infty} \mu(A_i), \tag{6}
\]

which means that \( \mu \) is countably additive and thus is a measure on \( \text{Cyl}(X) \), as required. \( \square \)

Although the above proposition allows us to introduce a measure on the semialgebra of elementary cylinder set, this semialgebra is “too small” a class of subsets of \( X \) to support the full machinery of probability theory. For this we need a \( \sigma \)-algebra, that is, a class of subsets of \( X \) that is closed under the complement and countable unions of its members. Such \( \sigma \)-algebra can be defined as an “extension” of \( \text{Cyl}(X) \). The smallest \( \sigma \)-algebra containing \( \text{Cyl}(X) \) will be called \( \sigma \)-algebra generated by \( \text{Cyl}(X) \). As it turns out, it is possible to extend a measure on semi-algebra to the \( \sigma \)-algebra generated by it, as the following theorem attests.

**Theorem 2.1 (Hahn-Kolmogorov)** Let \( \mu : \mathcal{D} \rightarrow [0, \infty] \) be a measure on semi-algebra \( \mathcal{D} \) of subsets of a set \( Y \). Then \( \mu \) can be extended to a measure on the \( \sigma \)-algebra generated by \( \mathcal{D} \).
This classic result has been first proved by M. Fréchet [9], and later by A. Kolmogorov [10] and H. Hahn [11]. One can find its contemporary proof in ref. [12]. The proof is based on construction of the outer measure $\mu^*$ determined by $\mu$, and then applying Carathéodory’s extension theorem. Since the proof bears little relevance to our subsequent considerations, it will be omitted here.

One can also show that the extension is unique if $\mu$ satisfies additional conditions. Without discussing this issue in full generality, we will only state that for probabilistic measures, that is, measures satisfying $\mu(X) = 1$, the extension is always unique [12]. In all subsequent considerations, we will assume that the measure is probabilistic, and the set of all probabilistic measures on the $\sigma$-algebra generated by elementary cylinder sets of $X$ will be denoted by $\mathcal{M}(X)$.

The Hahn-Kolmogorov Theorem coupled with Proposition 2.2 results in the following corollary, which summarizes our discussion.

**Corollary 2.1** Any finitely additive map $\mu : Cyl(X) \to [0, 1]$ satisfying $\mu(\emptyset) = 0$ and $\mu(X) = 1$ extends uniquely to a measure on the $\sigma$-algebra generated by elementary cylinder sets of $X$.

The last thing we need to do is to characterize finite additivity of maps on $Cyl(X)$ in somewhat simpler terms. Recall that $\mu : Cyl(X) \to [0, 1]$ is finitely additive if for every $B \in Cyl(X)$ and pairwise disjoint $A_i \in Cyl(X)$, $i = 1, 2, \ldots, m$ such that $B = \bigcup_{i=1}^m A_i$, we have $\mu(B) = \sum_{i=1}^m \mu(A_i)$. If $B$ is a cylinder set, when could it be a union of a finite number of other cylinder sets, pairwise disjoint? From the definition of the cylinder set, it is clear that if $B$ is a finite union of $A_i$, then each $A_i$ must be longer than $B$, and for each pair $(B, A_i)$ all fixed indices of $B$ must be matching. For $B = [b]_i$ this can happen in one of the following three situations:

\[
[b]_i = \bigcup_{a \in A^b} [ba]_i, \quad (7)
\]

\[
[b]_i = \bigcup_{a \in A^b} [ab]_{i-k}, \quad (8)
\]

\[
[b]_i = \bigcup_{a \in A^b, c \in A^t} [bac]_i. \quad (9)
\]

This means that we attach to $b$ a postfix word, a prefix word, or both, and take the union over all values of attached word(s). Note that all cylinder sets on the right hand side of each of the above equations are pairwise disjoint. If we want to test the map for countable additivity, it is thus sufficient to test it on cases described by equations (7–9).

**Proposition 2.3** The map $\mu : Cyl(X) \to [0, 1]$ is countably additive if and only if for all $[b]_i \in Cyl(X) \setminus X$,

\[
\mu([b]_i) = \sum_{a \in A} \mu([ba]_i) = \sum_{a \in A} \mu([ab]_{i-1}). \quad (10)
\]

**Proof:** Suppose that the map is countably additive. Applying additivity condition to eq. (7) and (8) with $a = a$ yields the desired result.
Now suppose that the double equality (10) holds. Applying it recursively \( k \) times we obtain
\[
\mu([b]_i) = \sum_{a_1 \in A} \ldots \sum_{a_k \in A} \mu([ba_1a_2 \ldots a_k]_i) = \sum_{a \in A^k} \mu([ba]_i),
\]
which implies additivity of \( \mu \) for the case covered by eq. (7). One can deal with cases covered by eqs. (8) and (9) in a similar fashion. The map \( \mu \) is thus countably additive on \( \text{Cyl}(X) \).

\[\square\]

Note that when \( b = \emptyset \), according to our convention, \([b]_i = X\), and eq. (10) reduces to
\[
\sum_{a \in A} \mu([a]_i) = 1,
\]
where we used the assumption that the measure is probabilistic, \( \mu(X) = 1 \).

### 3. Shift-invariant measure

In the previous section we demonstrated that any map \( \mu : \text{Cyl}(X) \rightarrow [0, 1] \) satisfying \( \mu(\emptyset) = 0 \), \( \mu(X) = 1 \) and conditions of eq. (10) extends uniquely to a measure on the \( \sigma \)-algebra generated by elementary cylinder sets of \( X \). We will now impose another condition on the map \( \mu : \text{Cyl}(X) \rightarrow [0, 1] \), namely translational invariance (also called shift-invariance), by requiring that, for all \( b \in A^* \), \( \mu([b]_i) \) is independent of \( i \). To simplify notation, we then define \( P : A^* \rightarrow [0, 1] \) as
\[
P(b) := \mu([b]_i).
\]

Values \( P(b) \) will be called block probabilities. Applying Proposition 2.3 and Hahn-Kolmogorov theorem to the case of shift-invariant \( \mu \) we obtain the following result.

**Theorem 3.1** Let \( P : A^* \rightarrow [0, 1] \) satisfy the conditions
\[
P(b) = \sum_{a \in A} P(ba) = \sum_{a \in G} P(ab) \quad \forall b \in A^*,
\]
\[
1 = \sum_{a \in G} P(a).
\]

Then \( P \) uniquely determines shift-invariant probability measure on the \( \sigma \)-algebra generated by elementary cylinder sets of \( X \).

The set of shift-invariant probability measures on the \( \sigma \)-algebra generated by elementary cylinder sets of \( X \) will be denoted by \( \mathcal{M}_\sigma(X) \). Conditions (14) and (15) are often called consistency conditions. It should be stressed, however, they are essentially equivalent to measure additivity conditions. Nevertheless, since the term “consistency conditions” is prevalent in the literature, we will use it in the subsequent considerations.

Since \( P \) uniquely determines the probability measure, we can use block probability values to define shift-invariant probability measure. Obviously, because of consistency conditions, block probabilities are not independent.
We will define $\mathbf{P}^{(k)}$ to be the column vector of all probabilities of blocks of length $k$ arranged in lexical order. For example, for $\mathcal{A} = \{0, 1\}$, these are
\[
\mathbf{P}^{(1)} = [P(0), P(1)]^T,
\]
\[
\mathbf{P}^{(2)} = [P(00), P(01), P(10), P(11)]^T,
\]
\[
\mathbf{P}^{(3)} = [P(000), P(001), P(010), P(011), P(100), P(101), P(110), P(111)]^T,
\]
\[
\ldots.
\]
Using this notation, eq. (14) can be written as
\[
\mathbf{P}^{(k-1)} = \mathbf{R}^{(k)} \mathbf{P}^{(k)} = \mathbf{L}^{(k)} \mathbf{P}^{(k)},
\] (16)
where $k > 1$ and where $\mathbf{L}^{(k)}$ and $\mathbf{R}^{(k)}$ are binary matrices with $N^{k-1}$ rows and $N^k$ columns. In order to describe structure of these matrices, let us denote identity matrix $N^{k-1} \times N^{k-1}$ by $\mathbf{I}$, and let $\mathbf{J}_m$ be a $N^{k-1} \times N^{k-1}$ matrix in which $m$-th row consist of all 1’s, and all other entries are 0. Then $\mathbf{L}^{(k)}$ and $\mathbf{R}^{(k)}$ can be written as
\[
\mathbf{L}^{(k)} = [\mathbf{I} \mathbf{I} \ldots \mathbf{I}]_N,
\] (17)
\[
\mathbf{R}^{(k)} = [\mathbf{J}_1 \mathbf{J}_2 \ldots \mathbf{J}_N].
\] (18)
For example, for $N = 3$, we have
\[
\mathbf{P}^{(2)} = [P(00), P(01), P(02), P(10), P(11), P(20), P(21), P(22)]^T,
\] (19)
\[
\mathbf{P}^{(1)} = [P(0), P(1), P(2)]^T,
\] (20)
and eq. (16) for $k = 2$ becomes
\[
\mathbf{P}^{(1)} = \begin{bmatrix}
1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 1
\end{bmatrix}, \quad \mathbf{P}^{(2)} = \begin{bmatrix}
1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 & 0 & 1 & 0 & 1
\end{bmatrix}, \quad \mathbf{P}^{(2)}. \] (21)
Dashed vertical lines illustrate partitioning of matrices $\mathbf{R}^{(3)}$ and $\mathbf{L}^{(3)}$ into blocks of $\mathbf{I}$ and $\mathbf{J}$ type.
We can now make two remarks about matrices $\mathbf{R}^{(k)}$ and $\mathbf{L}^{(k)}$. First of all, using eq. (16) recursively, we can express every $\mathbf{P}^{(m)}$ for $m \in [1, k]$ by $\mathbf{P}^{(k)}$,
\[
\mathbf{P}^{(m)} = \left( \prod_{i=m+1}^{k} \mathbf{L}^{(i)} \right) \mathbf{P}^{(k)}.
\] (22)
In the above, one could replace all (or only some) $\mathbf{L}$’s by $\mathbf{R}$’s, and the equation would remain valid.
Secondly, note that both $L^{(1)}$ and $R^{(1)}$ are single row matrices with all $N$ entries equal to 1. This implies that the product $L^{(1)}L^{(2)}$ is a single row matrix with all $N^2$ entries equal to 1, and, in general, for any $k \geq 1$,

$$\prod_{i=1}^{k} L^{(i)} = \begin{bmatrix} 1 & 1 & \ldots & 1 \end{bmatrix}_{N^k}. \quad (23)$$

Again, one could replace here all (or some) $L$’s by $R$’s, and the equation would remain valid. As a consequence of this, normalization condition (15) can be written as $L^{(1)}P^{(1)} = 1$, or, replacing $P^{(1)}$ by $L^{(2)}P^{(2)}$, as $L^{(1)}L^{(2)}P^{(2)} = 1$, etc. In general, we can write the normalization condition in the form

$$\left( \prod_{i=1}^{k} L^{(i)} \right) P^{(k)} = 1, \quad (24)$$

which, of course, is equivalent to

$$\sum_{i=1}^{N^k} P^{(k)} = 1. \quad (25)$$

Naturally, this was to be expected, since it is a consequence of measure additivity and the fact that

$$\bigcup_{b \in A^k} [b]_i = X. \quad (26)$$

After making the above remarks about consistency conditions and their matrix form, let us turn our attention to the following problem. In order to fully describe a shift-invariant probability measure one needs to know all block probabilities $P^{(i)}$ with $i = 1, 2, \ldots$, and make sure that they satisfy consistency conditions. In practical applications, however, it is often impossible to know all block probabilities, and instead one considers only truncated sequence of block probabilities $P^{(i)}$ for $i = 1, 2, \ldots, k$. It is then important to know how many of these are truly independent? The next proposition answers this question.

**Proposition 3.1** Among all block probabilities constituting components of $P^{(1)}, P^{(2)}, \ldots, P^{(k)}$ only $(N - 1)N^{k-1}$ are linearly independent.

**Proof:** Let us first note that vector $P^{(i)}$ has $N^i$ components. Collectively, in $P^{(1)}, P^{(2)}, \ldots, P^{(k)}$ we have, therefore, $\sum_{i=1}^{k} N^i = (N^{k+1} - N)/(N - 1)$ block probabilities. However, since all $P^{(i)}, i \in [1, k)$, can be expressed in terms of $P^{(k)}$ with the help of eq. (22), we can treat all of $P^{(1)}, P^{(2)}, \ldots, P^{(k-1)}$ as dependent. This leaves us with $P^{(k)}$ with $N^k$ components. However, we also have

$$L^{(k)}P^{(k)} = R^{(k)}P^{(k)}. \quad (27)$$

Matrices in the above have $N^{k-1}$ rows, thus we have $N^{k-1}$ equations for $N^k$ variables. Are they all these equations independent? Both $L$ and $R$ have the property that sum of each of their columns is 1. Thus if we add all equations of (27), we obtain identity $\sum P^{(k)} = \sum P^{(k)}$, meaning that the number of independent equations in eq. (27) is $N^{k-1} - 1$. All of this takes care of consistency conditions (14), but we also need to consider normalization condition (15) which, as remarked earlier, can be written in equivalent form as equation

8
involving components of $\mathbf{P}^{(k)}$, that is, eq. (25). This additional equation increases our previously obtained number of independent equations back to $N^k-1$. In the end, the number of independent block probabilities, equal to number of variables minus number of independent equations, is $N^k - N^{k-1} = (N - 1)N^{k-1}$. □

Once we know how many independent block probabilities are there, we can express the remaining block probabilities in terms of them. We need to choose which block probabilities we declare to be independent. The following proposition describes a natural choice. Before we state it, we need to introduce some additional notation. As explained in the proof of Proposition 3.1 in the system of equations $\mathbf{R}^{(k)}\mathbf{P}^{(k)} = \mathbf{L}^{(k)}\mathbf{P}^{(k)}$ only $N^{k-1} - 1$ equations are independent. We can, therefore, remove one of them, for example, the last equation, and replace it by normalization condition $\sum \mathbf{P}^{(k)} = 1$. This will result in

$$
\mathbf{M}^{(k)}\mathbf{P}^{(k)} = \begin{bmatrix}
0 \\
\vdots \\
0 \\
1
\end{bmatrix},
$$

(28)

where the matrix $\mathbf{M}^{(k)}$ has been obtained from $\mathbf{R}^{(k)} - \mathbf{L}^{(k)}$ by setting every entry in the last row of $\mathbf{R}^{(k)} - \mathbf{L}^{(k)}$ to 1. Let us now partition $\mathbf{M}^{(k)}$ into two submatrices, so that the first $N^k - N^{k-1}$ columns of it are called $\mathbf{A}^{(k)}$, and the remaining $N^{k-1}$ columns are called $\mathbf{B}^{(k)}$, so that

$$
\mathbf{M}^{(k)} = [\mathbf{A}^{(k)} \mathbf{B}^{(k)}].
$$

(29)

If we recall definitions of $\mathbf{L}^{(k)}$ and $\mathbf{R}^{(k)}$ in eqs. (17) and (18), we can easily verify that

$$
\mathbf{B}^{(k)} = \begin{bmatrix}
-1 & 0 & \cdots & 0 \\
0 & -1 & \ddots & \\
\vdots & \ddots & \ddots & \\
1 & 1 & 1 & 1
\end{bmatrix},
$$

(30)

so that $\mathbf{B}^{(k)}$ can be constructed from zero $N^{k-1} \times N^{k-1}$ matrix by placing $-1$’s on the diagonal, and then filling the last row with $1$’s. The structure of matrix $\mathbf{A}^{(k)}$ is a bit more complicated,

$$
\mathbf{A}^{(k)} = [\mathbf{J}_1 \mathbf{J}_2 \ldots \mathbf{J}_{N-1}] + \underbrace{[\mathbf{B}^{(k)} \mathbf{B}^{(k)} \ldots \mathbf{B}^{(k)}]}_{N-1},
$$

(31)

where, as already defined, $\mathbf{J}_m$ is an $N^{k-1} \times N^{k-1}$ matrix in which $m$-th row consist of all $1$’s, and all other entries are equal to $0$.

**Proposition 3.2** Let $\mathbf{P}^{(k)}$ be partitioned into two subvectors, $\mathbf{P}^{(k)} = (\mathbf{P}_{\text{Top}}, \mathbf{P}_{\text{Bot}})$, where $\mathbf{P}_{\text{Top}}$ contains first $N^k - N^{k-1}$ entries of $\mathbf{P}^{(k)}$, and $\mathbf{P}_{\text{Bot}}$ the remaining $N^{k-1}$ entries. Then

$$
\mathbf{P}_{\text{Bot}}^{(k)} = \begin{bmatrix}
0 \\
\vdots \\
0 \\
1
\end{bmatrix} - (\mathbf{B}^{(k)})^{-1} \mathbf{A}^{(k)} \mathbf{P}_{\text{Top}}^{(k)}.
$$

(32)
Proof: we want to solve

\[
\begin{bmatrix}
A^{(k)} & B^{(k)}
\end{bmatrix}
\begin{bmatrix}
P_{\text{Top}}^{(k)} \\
P_{\text{Bot}}^{(k)}
\end{bmatrix}
= \begin{bmatrix}
0 \\
\vdots \\
0 \\
1
\end{bmatrix}
\]  

(33)

for \(P_{\text{Bot}}^{(k)}\). Denoting the vector on the right hand side by \(c\) and performing block multiplication we obtain \(A^{(k)} P_{\text{Top}}^{(k)} + B^{(k)} P_{\text{Bot}}^{(k)} = c\). The matrix \(B^{(k)}\) is always invertible, and has the property \((B^{(k)})^{-1} c = c\). This leads to \(P_{\text{Bot}}^{(k)} = c - (B^{(k)})^{-1} A^{(k)} P_{\text{Top}}^{(k)}\), as desired. □

**Corollary 3.1** Among block probabilities constituting components of \(P^{(1)}, P^{(2)}, \ldots, P^{(k)}\), we can treat first \(N^k - N^{k-1}\) entries of \(P^{(k)}\) as independent variables. Remaining components of \(P^{(k)}\) can be obtained by using eq. (32), while \(P^{(1)}, P^{(2)}, \ldots, P^{(k-1)}\) can be obtained by eq. (22).

Representation of all blocks \(P^{(1)}, P^{(2)}, \ldots, P^{(k)}\) by first \(N^k - N^{k-1}\) entries of \(P^{(k)}\) will be called long block representation. As an example of this, let us consider the case of \(A = \{0, 1, 2\}\) (\(N = 3\)) and \(P^{(1)}, P^{(2)}, P^{(3)}\). We have \(3^3 - 3^2 = 18\) independent block probabilities, all of length 3. These are

\[
\{ P(000), P(001), P(002), P(010), P(011), P(012), P(020), P(021), P(022), P(100), P(101), P(102), P(110), P(111), P(112), P(120), P(121), P(122) \}.
\]

Remaining 21 block probabilities, expressible in terms of the above, are

\[
\{ P(200), P(201), P(202), P(210), P(211), P(212), P(220), P(221), P(222), P(00), P(01), P(02), P(10), P(11), P(12), P(20), P(21), P(22), P(0), P(1), P(2) \}.
\]

Since there are there are total \(\sum_{i=1}^{k} N^i = (N^{k+1} - N)/(N - 1)\) block probabilities in \(P^{(1)}, P^{(2)}, \ldots, P^{(k)}\), the fraction of independent block probabilities among all block probabilities up to length \(k\) is

\[
\text{Ind}(N, k) := \frac{(N - 1)(N^k - N^{k-1})}{N^{k+1} - N}.
\]

(34)

For fixed \(N\), \(\text{Ind}(N, k)\) decreases as a function of \(k\), and tends to the limit

\[
\lim_{k \to \infty} \text{Ind}(N, k) = \frac{(N - 1)^2}{N^2}
\]

(35)

The above reaches minimum 1/4 at \(N = 2\), thus \(\text{Ind}(N, k) > 1/4\) for all \(k \geq 1, N > 1\). This means that the long block expression is most “economical” for the binary alphabet. For
example, for $N = 2$ and $k = 3$, among $\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \mathbf{P}^{(3)}$ we have only 4 independent blocks, $P(000), P(001), P(010)$ and $P(011)$. Remaining 10 probabilities can be expressed as follows,

$$
\begin{bmatrix}
P(100) \\
P(101) \\
P(110) \\
P(111)
\end{bmatrix} = 
\begin{bmatrix}
P(001) \\
-P(001) + P(010) + P(011) \\
P(011) \\
1 - P(000) - P(001) - 2P(010) - 3P(011)
\end{bmatrix},
\begin{bmatrix}
P(00) \\
P(01) \\
P(10) \\
P(11)
\end{bmatrix} = 
\begin{bmatrix}
P(000) + P(001) \\
P(010) + P(011) \\
1 - P(000) - P(001) - 2P(010) - 2P(011)
\end{bmatrix},
\begin{bmatrix}
P(0) \\
P(1)
\end{bmatrix} = 
\begin{bmatrix}
P(000) + P(001) + P(010) + P(011) \\
1 - P(000) - P(001) - P(010) - P(011)
\end{bmatrix}.
$$

(36)

Of course, the long block representation is not the only one possible. We will describe below yet another representation, which is in some sense complementary to the the long block one. It declares as independent blocks of shortest possible length, thus it will be called *short block representation*.

It is constructed as follows. We start, as before, with block probabilities $\mathbf{P}^{(1)}, \mathbf{P}^{(2)}, \ldots, \mathbf{P}^{(k)}$, and we arrange each of the vectors $\mathbf{P}^{(i)}$ in a vertical column. Example of this is shown in Figure[I]. In each vector $\mathbf{P}^{(i)}$, we put aside last $N^{i-1}$ entries, and in what remains, we underline every $N$-th entry, starting from the top. Entries which are still left are framed (cf. Figure[I]), and those we declare to be independent. It is straightforward to verify that we have $N^{k} - N^{k-1}$ independent entries, as we should. Now how do we express dependent entries in terms of independent ones? In each vector, starting from the left, we replace each underlined entry by a linear combinations of boxed entries from the same column and (possibly) entries from the column on the left hand side, by following the path which starts with $\rightarrow$ arrow and which ends at the underlined entry in question. For example, for $P(02)$, such path is $P(0) \rightarrow P(00) \rightarrow P(01) \rightarrow P(02)$. Labels above arrows indicate how the equation is to be constructed, in this case

$$
P(0) - P(00) - P(01) = P(02).
$$

(37)

All arrows are labeled with “$-$”, except those which point toward underlined entries, which are labeled with “$=$”.

Once we are done with all underlined entries in a given vector, we express all entries marked as $\mathbf{P}_{Bot}$ by $\mathbf{P}_{Top}$, using eq. (32). We then move to the next vector on the right and repeat the same procedure, until all vectors are dealt with. By inspecting Figure[I] the reader can verify that the short block representation utilizes short blocks as much possible, and that, in fact, it is not possible to declare a larger number of short blocks as independent.

In order to describe the above algorithm in a more formal way, let us define vector of *admissible entries* for short block representation, $\mathbf{P}^{(k)}_{adm}$, as follows. Let us take vector $\mathbf{P}^{(k)}$ in which block probabilities are arranged in lexicographical order, indexed by an index $i$ which runs from 1 to $N^{k}$. Vector $\mathbf{P}^{(k)}_{adm}$ consists of all entries of $\mathbf{P}^{(k)}$ for which the index $i$ is not
Figure 1: Generation of short block representation for $N = 3$ and $\mathbf{P}^{(k)}$ for $k = 1, 2, 3$. Independent block probabilities are boxed, while dependent block probabilities obtained from probabilities of shorter blocks are underlined.
divisible by \( N \) and for which \( i < N^k - N^{k-1} \). For example, for \( N = 3 \) and \( k = 2 \) we have

\[
\mathbf{P}^{(2)} = [P(00), P(01), P(02), P(10), P(11), P(12), P(20), P(21), P(22)]^T,
\]

and we need to select entries with \( i \) not divisible by 3 and \( i < 6 \), which leaves \( i = 1, 2, 4, 5 \), hence

\[
\mathbf{P}^{(2)}_{adm} = [P(00), P(01), P(10), P(11)]^T.
\]

Vector of independent block probabilities in short block representation is now defined as

\[
\mathbf{P}_{short}^{(k)} = \begin{bmatrix}
\mathbf{P}^{(1)}_{adm} \\
\mathbf{P}^{(2)}_{adm} \\
\vdots \\
\mathbf{P}^{(k)}_{adm}
\end{bmatrix},
\]

(38)

For \( N = 3 \) and \( k = 2 \), elements of \( \mathbf{P}^{(3)}_{short} \) are shown in Figure 1 in red color. Note that the length of \( \mathbf{P}^{(k)}_{short} \) is the same as \( \mathbf{P}^{(k)}_{Top} \). We can, therefore, transform one into the other by a linear transformation. The form of this transformation can be deduced from Figure 1. Consider, for example, \( k = 2 \), so that \( \mathbf{P}^{(2)}_{Top} = [P(00), P(01), P(02), P(10), P(11), P(12)]^T \) and \( \mathbf{P}^{(2)}_{adm} = [P(00), P(01), P(10), P(11)]^T, \mathbf{P}^{(1)}_{bot} = \mathbf{P}^{(1)}_{adm} = [P(0), P(1)]^T. \) From Figure 1, we read

\[
\begin{align*}
P(00) &= P(00), \\
P(01) &= P(01), \\
P(02) &= P(0) - P(00) - P(01), \\
P(10) &= P(00), \\
P(11) &= P(01), \\
P(12) &= P(1) - P(10) - P(11),
\end{align*}
\]

where, if an element \( P(b) \) of \( \mathbf{P}^{(2)}_{Top} \) was admissible, we wrote \( P(b) = P(b) \), and if it was admissible, we expressed it in terms of probabilities of shorter blocks. The above can be written as

\[
\mathbf{P}^{(2)}_{Top} = \begin{bmatrix}
0 & 0 \\
0 & 0 \\
1 & 0 \\
0 & 0 \\
0 & 0 \\
0 & 1
\end{bmatrix} \mathbf{P}^{(1)}_{adm} + \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
-1 & -1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & -1 & -1
\end{bmatrix} \mathbf{P}^{(2)}_{adm}, \tag{40}
\]

This expresses \( \mathbf{P}^{(2)}_{Top} \) in terms of \( \mathbf{P}^{(1)}_{adm} \) and \( \mathbf{P}^{(2)}_{adm} \), that is, in terms of \( \mathbf{P}^{(2)}_{short} \). One can similarly show that for general \( k > 1 \),

\[
\mathbf{P}^{(k)}_{Top} = C^{(k)} \mathbf{P}^{(k-1)}_{Top} + D^{(k)} \mathbf{P}^{(k)}_{adm}, \tag{41}
\]
where
\[
C^{(k)} = \text{diag}(e_N, e_N, \ldots, e_N), \quad e_N = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix}
\]

\[
D^{(k)} = \text{diag}(D_N, D_N, \ldots, D_N), \quad D_N = \begin{bmatrix} I_{N-1} \\ -1, -1, \ldots, -1 \end{bmatrix}
\]

Note that \(C^{(k)}\) has \(N^k - N^{k-1}\) rows and \(N^{k-1} - N^{k-2}\) columns, while \(D^{(k)}\) has \(N^k - N^{k-1}\) rows and \((N^{k-1} - N^{k-2})(N-1)\) columns. Applying eq. (44) \(k - 1\) times recursively, one obtains, for \(k > 2\),

\[
P^{(k)}_{\text{Top}} = C^{(k)} C^{(k-1)} \ldots C^{(2)} P^{(1)}_{\text{adm}} + \sum_{i=2}^{k-1} C^{(k)} C^{(k-1)} \ldots C^{(i+1)} D^{(i)} P^{(i)}_{\text{adm}} + D^{(k)} P^{(k)}_{\text{adm}}.
\]

When \(k = 2\) no recursion is needed, as eq. (44) becomes

\[
P^{(2)}_{\text{Top}} = C^{(2)} P^{(1)}_{\text{adm}} + D^{(2)} P^{(2)}_{\text{adm}},
\]

and for \(k = 1\) we simply have

\[
P^{(1)}_{\text{Top}} = P^{(1)}_{\text{adm}} = P^{(1)}_{\text{short}}.
\]

If we define

\[
M^{(k)}_{\text{short}} = \begin{cases} 
\left[ C^{(k)} C^{(k-1)} \ldots C^{(2)}, C^{(k)} C^{(k-1)} \ldots C^{(i+1)} D^{(i)}, D^{(k)} \right], & k > 2 \\
[ C^{(2)}, D^{(2)} ], & k = 2 \\
I_{N-1}, & k = 1
\end{cases}
\]

then equations (44), (46) can be written as

\[
P^{(k)}_{\text{Top}} = M^{(k)}_{\text{short}} P^{(k)}_{\text{short}}.
\]

**Proposition 3.3** Among block probabilities constituting components of \(P^{(1)}, P^{(2)}, \ldots, P^{(k)}\), we can treat entries of \(P^{(k)}_{\text{short}}\) as independent variables. One can express first \(N^k - N^{k-1}\) components of \(P^{(k)}\) by \(P^{(k)}_{\text{short}}\) by means of eq. (48). Remaining components of \(P^{(k)}\) can be obtained by using eq. (44), while \(P^{(1)}, P^{(2)}, \ldots, P^{(k-1)}\) can be obtained by eq. (42).

Let us now apply the procedure described above to the \(N = 2\) and \(k = 3\) case, the same as we already considered for long block representation. Among components of \(P^{(1)}, P^{(2)}\) and \(P^{(3)}\), we have only four independent block probabilities, \(P^{(3)}_{\text{short}} = [P(0), P(00), P(000), P(010)]^T\), and 10 dependent probabilities. We first partition \(P^{(3)}\) into two subvectors, \(P^{(3)}_{\text{Top}} = [P(000),\)
\[ P(001), P(010), P(011) \] and \( P_{Bot}^{(3)} = [P(100), P(101), P(111)] \). Eq. \([48]\) takes the form
\[
P_{Top}^{(3)} = \begin{bmatrix} P(000) \\ P(001) \\ P(010) \\ P(011) \end{bmatrix} = M_{short}^{(3)} P_{short}^{(3)} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & -1 & 0 & -1 \end{bmatrix} \begin{bmatrix} P(0) \\ P(00) \\ P(000) \\ P(010) \end{bmatrix}. \tag{49}
\]
Components of \( P_{Bot}^{(3)} \) can be obtained from eq. \([32]\),
\[
\begin{bmatrix} P(100) \\ P(101) \\ P(110) \\ P(111) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix} - \begin{bmatrix} 0 & -1 & 0 & 0 \\ 0 & 1 & -1 & -1 \\ 0 & 0 & 0 & -1 \\ 1 & 1 & 2 & 3 \end{bmatrix} \begin{bmatrix} P(000) \\ P(001) \\ P(010) \\ P(011) \end{bmatrix}, \tag{50}
\]
and we can use eq. \([49]\) again to replace \([P(000), P(001), P(010), P(011)]\) on the right hand side by \( M_{short}^{(3)} P_{short}^{(3)} \). Equations \([49]\) and \([50]\), therefore, yield all components of \( P^{(3)} \). By applying eq. \([22]\) we can obtain \( P^{(2)} \) and of \( P^{(1)} \). This will yield the following 10 dependent blocks probabilities expressed in terms of elements of \( P_{short}^{(3)} \):
\[
\begin{bmatrix} P(001) \\ P(011) \\ P(100) \\ P(101) \\ P(110) \\ P(111) \end{bmatrix} = \begin{bmatrix} P(00) - P(000) \\ P(00) - P(000) \\ P(00) - P(000) \\ P(00) - 2P(00) + P(000) \\ P(00) - P(00) - P(010) \\ 1 - 3P(0) + 2P(00) + P(010) \end{bmatrix}.
\]
We can see that the resulting expressions are shorter than in the case of long block representation given by eq. \([30]\). Indeed, the short block representation is more "natural" and often helps to gain insight into the properties of the probability measure it describes. We will see this when this representation is used to simplify local structure theory equations.

4. Bayesian Extension

From what we have seen so far, it is clear that the knowledge of \( P^{(k)} \) is enough to determine all \( P^{(i)} \) with \( i < k \). What about \( i > k \)? Obviously, since the number of independent components in \( P^{(i)} \) is greater than in \( P^{(k)} \) for \( i > k \), there is no hope to determine \( P^{(i)} \) using only \( P^{(k)} \). It is possible, however, to approximate longer block probabilities by shorter block probabilities using the idea of Bayesian extension.
Suppose now that we want to approximate \( P(a_1a_2\ldots a_{k+1}) \) by \( P(a_1a_2\ldots a_k) \). One can say that by knowing \( P(a_1a_2\ldots a_k) \) we know how values of individual symbols in a block are correlated providing that symbols are not farther apart than \( k - 1 \). We do not know, however, anything about correlations on the larger length scale. The only thing we can do in this situation is to simply neglect these higher length correlations, and assume that if a block of length \( k \) is extended by adding another symbol to it on the right, then the the conditional probability of finding a particular value of that symbol does not significantly depend on the left-most symbol, i.e.,

\[
\frac{P(a_1a_2\ldots a_{k+1})}{P(a_1\ldots a_k)} \approx \frac{P(a_2\ldots a_{k+1})}{P(a_2\ldots a_k)}.
\] (52)

This produces the desired approximation of \( k + 1 \) block probabilities by \( k \)-block and \( k - 1 \) block probabilities,

\[
P(a_1a_2\ldots a_{k+1}) \approx \frac{P(a_1\ldots a_k)P(a_2\ldots a_{k+1})}{P(a_2\ldots a_k)},
\] (53)

where we assume that the denominator is positive. If the denominator is zero, then we take \( P(a_1a_2\ldots a_{k+1}) = 0 \). In order to avoid writing separate cases for denominator equal to zero, we define “thick bar” fraction as

\[
a_b := \begin{cases} \frac{a}{b} & \text{if } b \neq 0 \\ 0 & \text{if } b = 0. \end{cases}
\] (54)

Note that eq. (53) only makes sense if \( k > 1 \). For \( k = 1 \), the approximation is

\[
P(a_1a_2) \approx P(a_1)P(a_2).
\] (55)

Again, in order to avoid writing the \( k = 1 \) case separately, we adopt notational convention that

\[
P(a_m\ldots a_n) = 1 \text{ whenever } n > m,
\] (56)

and then eq. (53) remains valid even for \( k = 1 \). Using notational conventions given in eq. (54) and (56) and applying our approximation recursively \( m \) times we can express \( k + m \) block probabilities in terms of \( k \) and \( k - 1 \)-block probabilities,

\[
P(a_1a_2\ldots a_{k+m}) \approx \frac{\prod_{i=1}^{m+1} P(a_i\ldots a_{i+k-1})}{\prod_{i=1}^{m} P(a_{i+1}\ldots a_{i+k-1})}.
\] (57)

Note that if we want, we can write the right hand side of the above in terms of only \( k \)-block probabilities, by substituting in the denominator

\[
P(a_{i+1}\ldots a_{i+k-1}) = \sum_{b \in A} P(a_{i+1}\ldots a_{i+k-1}b).
\] (58)
Proposition 4.1 Let $\mu \in \mathcal{M}_\sigma(X)$ be a measure with associated block probabilities $P : \mathcal{A}^* \to [0,1]$, $P(b) = \mu([b]_i)$ for all $i \in \mathbb{Z}$ and $b \in \mathcal{A}^*$. For $k > 0$, define $\tilde{P} : \mathcal{A}^* \to [0,1]$ such that

$$
\tilde{P}(a_1a_2 \ldots a_p) = \begin{cases} 
P(a_1a_2 \ldots a_p) & \text{if } p \leq k, \\
\frac{\prod_{i=1}^{p-k+1} P(a_i \ldots a_{i+k-1})}{\prod_{i=1}^{p-k} P(a_{i+1} \ldots a_{i+k-1})} & \text{otherwise.}
\end{cases} \tag{59}
$$

Then $\tilde{P}$ determines a shift-invariant probability measure $\tilde{\mu}^{(k)} \in \mathcal{M}_\sigma(X)$, to be called Bayesian approximation of $\mu$ of order $k$.

**Proof.** If $b = b_1b_2 \ldots b_n$, we will denote subblocks of $b$ by $b_{[i,j]} = b_ib_{i+1} \ldots b_j$. Using Theorem 3.1, all we need to do is to show that conditions (14) and (15) are satisfied by $\tilde{P}$. The second one holds for $\tilde{P}$, because it obviously holds for $P$. For the same reason eq. (14) holds for block $b$ of length up to $k - 1$. For $b = b_1b_2 \ldots b_p$, $p \geq k$, we have

$$
\sum_{a \in \mathcal{A}} \tilde{P}(ba) = \sum_{a \in \mathcal{A}} \frac{\prod_{i=1}^{p-k+1} P(b_{[i,i+k-1]}) \cdot P(b_{[p-k+2,p]}a)}{\prod_{i=1}^{p-k} P(b_{[i+1,i+k-1]}) \cdot P(b_{[p-k+2,p]})} = \frac{\prod_{i=1}^{p-k+1} P(b_{[i,i+k-1]})}{\prod_{i=1}^{p-k} P(b_{[i+1,i+k-1]})} \sum_{a \in \mathcal{A}} P(b_{[p-k+2,p]}a) = \frac{\prod_{i=1}^{p-k+1} P(b_{[i,i+k-1]})}{\prod_{i=1}^{p-k} P(b_{[i+1,i+k-1]})} \cdot P(b_{[p-k+2,p]}) = \tilde{P}(b). \tag{60}
$$

One can similarly prove that $\sum_{a \in \mathcal{A}} \tilde{P}(ab) = \tilde{P}(b)$. □

When there exists $k$ such that Bayesian approximation of $\mu$ of order $k$ is equal to $\mu$, we call $\mu$ a Markov measure or a finite block measure of order $k$. The space of Markov measures of order $k$ will be denoted by $\mathcal{M}^{(k)}(X)$,

$$
\mathcal{M}^{(k)}(X) = \{ \mu \in \mathcal{M}_\sigma(X) : \mu = \tilde{\mu}^{(k)} \}. \tag{61}
$$

It is often said that the Bayesian approximation “maximizes entropy”. In order to state this property in a formal way, let us define entropy density of shift-invariant measure $\mu \in \mathcal{M}_\sigma(X)$ as

$$
h(\mu) = \lim_{n \to \infty} -\frac{1}{n} \sum_{b \in \mathcal{A}^n} P(b) \log P(b), \tag{62}
$$

where, as usual, $P(b) = \mu([b]_i)$ for all $i \in \mathbb{Z}$ and $b \in \mathcal{A}^*$. The following two propositions and the main ideas behind their proofs are due to M. Fannes and A. Verbeure [8].

**Proposition 4.2** For any $\mu \in \mathcal{M}_\sigma(X)$, the entropy density of the $k$-th order Bayesian approximation of $\mu$ is given by

$$
h(\tilde{\mu}^{(k)}) = \sum_{a \in \mathcal{A}^{k-1}} P(a) \log P(a) - \sum_{a \in \mathcal{A}^k} P(a) \log P(a). \tag{63}
$$
Proof: Since we are interested in \( n \to \infty \) limit, let us consider \( n > k \). Then

\[
\sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) = \sum_{b \in A^n} \tilde{P}(b) \log \frac{\prod_{i=1}^{n-k+1} P(b_{[i,i+k-1]})}{\prod_{i=1}^{n-k} P(b_{[i+1,i+k-1]})}
\]

\[
= \sum_{b \in A^n} \tilde{P}(b) \sum_{i=1}^{n-k+1} \log P(b_{[i,i+k-1]}) - \sum_{b \in A^n} \tilde{P}(b) \sum_{i=1}^{n-k} \log P(b_{[i+1,i+k-1]})
\]

(64)

For any \( i \in [1, n - k + 1] \),

\[
\sum_{b \in A^n} \tilde{P}(b) \log P(b_{[i,i+k-1]}) =
\]

\[
= \sum_{b_{[1,i-1]} \in A^{i-1}} \sum_{b_{[i,i+k-1]} \in A^k} \sum_{b_{[i+k,n]} \in A^{n-i-k+1}} \tilde{P}(b_{[1,i-1]} b_{[i,i+k-1]} b_{[i+k,n]}) \log P(b_{[i,i+k-1]})
\]

\[
= \sum_{a \in A^k} \tilde{P}(a) \log P(a) = \sum_{a \in A^k} P(a) \log P(a),
\]

(65)

and, by the same reasoning, any \( i \in [1, n - k] \),

\[
\sum_{b \in A^n} \tilde{P}(b) \log P(b_{[i+1,i+k-1]}) = \sum_{a \in A^{k-1}} P(a) \log P(a).
\]

(66)

Using this, eq. (64) becomes

\[
\sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) =
\]

\[
(n - k + 1) \sum_{a \in A^k} P(a) \log P(a) - (n - k) \sum_{a \in A^{k-1}} P(a) \log P(a).
\]

(67)

Dividing this by \(-n\) and taking the limit \( n \to \infty \) we obtain the desired expression. \( \square \)

Theorem 4.1 For any \( \mu \in \mathfrak{M}_\sigma(X) \) and any \( k > 0 \), the entropy density of \( \mu \) does not exceed the entropy density of its \( k \)-th order Bayesian approximation,

\[
h(\mu) \leq h(\tilde{\mu}^{(k)}).
\]

(68)

Proof: Let

\[
H_n(\mu) = - \sum_{b \in A^n} P(b) \log P(b),
\]

(69)

\[
H_n(\tilde{\mu}^{(k)}) = - \sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b),
\]

(70)

(71)
We will use convexity of \( f(x) = x \log x \),
\[
x \log x - y \log y \leq (x - y)(1 + \log x).
\] (72)
Applying this inequality to \( S_n(\mu) - S_n(\mu^{(k)}) \) for \( n > k \) we obtain
\[
H_n(\mu) - H_n(\mu^{(k)}) = \sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) - \sum_{b \in A^n} P(b) \log P(b)
\leq \sum_{b \in A^n} \left( \tilde{P}(b) - P(b) \right) \left( 1 + \log \tilde{P}(b) \right)
= \sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) - \sum_{b \in A^n} P(b) \log \tilde{P}(b),
\] (73)
where we used the fact that \( \sum_{b \in A^n} \tilde{P}(b) = \sum_{b \in A^n} P(b) = 1 \). Note that we already computed the value of \( \sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) \) (cf. eq. [67]). Also note that nothing would change in the derivation of eq. [67] if we were computing \( \sum_{b \in A^n} P(b) \log \tilde{P}(b) \) instead, meaning that
\[
\sum_{b \in A^n} \tilde{P}(b) \log \tilde{P}(b) = \sum_{b \in A^n} P(b) \log \tilde{P}(b).
\] (74)
We therefore obtain
\[
H_n(\mu) - H_n(\mu^{(k)}) \leq 0.
\] (75)
Dividing this by \( n \) and taking the limit \( n \to \infty \) we obtain inequality [68]. \( \square \)

Let \( \mu, \mu_n \in \mathcal{M}(X) \). If \( \int_X f d\mu_n \to \int_X f d\mu \) as \( n \to \infty \) for every bounded, continuous real function \( f \) on \( X \), we say that \( \mu_n \) converges weakly to \( \mu \) and write \( \mu_n \Rightarrow \mu \). Proof of the following useful criterion of weak convergence, originally due to Kolmogorov and Prohorov [13], can be found in [14].

**Theorem 4.2** Let \( U \) be a subclass of the smallest \( \sigma \)-algebra containing all open sets of \( X \) such that (i) \( U \) is closed under the formation of finite intersections and (ii) each open set in \( X \) is a finite or countable union of elements of \( U \). If \( \mu_n(A) \to \mu(A) \) for every \( A \in U \), then \( \mu_n \Rightarrow \mu \).

The subclass \( U \) satisfying hypothesis of the above theorem is called convergence determining class. It is easy to verify that \( Cyl(X) \) is a convergence determining class for measures in \( \mathcal{M}(X) \), hence the following proposition.

**Proposition 4.3** The sequence of \( k \)-th order Bayesian approximations of \( \mu \in \mathcal{M}_\sigma(X) \) weakly converges to \( \mu \) as \( k \to \infty \).

**Proof:** Let \( n > 0, b \in A^n \) and let \( \tilde{P}_k(b) = \tilde{\mu}^{(k)}([b]_0), P(b) = \mu([b]_0) \). Since for \( k \geq n \) \( \tilde{P}_k(b) = P(b) \), we obviously have \( \lim_{k \to \infty} \tilde{P}_k(b) = P(b) \). Theorem 4.2 coupled with the fact that \( Cyl(X) \) is a convergence determining class leads to the conclusion that \( \tilde{\mu}^{(k)} \Rightarrow \mu \). \( \square \)
5. Cellular automata

Let $w : \mathcal{A} \times \mathcal{A}^{2r+1} \rightarrow [0, 1]$, whose values are denoted by $w(a|b)$ for $a \in \mathcal{A}$, $b \in \mathcal{A}^{2r+1}$, satisfying $\sum_{a \in \mathcal{A}} w(a|b) = 1$, be called local transition function of radius $r$, and its values will be called local transition probabilities. Probabilistic cellular automaton with local transition function $w$ is a map $F : \mathfrak{M}(X) \rightarrow \mathfrak{M}(X)$ defined as

$$(F\mu)([b]_i) = \sum_{a \in \mathcal{A}^{[b]+2r}} w(a|b)\mu([a]_{i-r}) \text{ for all } i \in \mathbb{Z}, b \in \mathcal{A}^*,$$

where we define

$$w(a|b) = \prod_{j} w(a_j|b_jb_{j+1}\ldots b_{j+2r}).$$

When the function $w$ takes values in the set $\{0, 1\}$, the corresponding cellular automaton is called deterministic CA.

For any probabilistic measure $\mu \in \mathfrak{M}(X)$, we define the orbit of $\mu$ under $F$ as

$$\{F^n\mu\}_{n=0}^\infty.$$  

In general, it is very difficult to compute $F^n\mu$ directly, and no general method for doing this is known. To see the source of the difficulty, let us take $\mathcal{A} = \{0, 1\}$ and let us consider the example of rule 14, for which local transitions probabilities are given by

$$w(1|000) = 0, \ w(1|001) = 1, \ w(1|010) = 1, \ w(1|011) = 1,$$
$$w(1|100) = 0, \ w(1|101) = 0, \ w(1|110) = 0, \ w(1|111) = 0.$$  

Let us further suppose that we want to compute orbit of a shift-invariant Bernoulli measure $\mu_{1/2}$, such that for any block $b \in \mathcal{A}^*$, $\mu_{1/2}([b]) = (1/2)^{|b|}$. If we, for example, consider blocks $b$ of length 2, then, defining $P_n(b) = (F^n\mu_b)([b])$, equation (76) becomes

$$P_{n+1}(0) = 1 - P_n(0) + P_n(00),$$
$$P_{n+1}(00) = 1 - 2P_n(0) + P_n(00) + P_n(000).$$

It is obvious that this system of equations cannot be iterated over $n$, because on the left hand side we have probabilities of blocks of length 2, and on the right hand side – probabilities of blocks of length 4. Of course, not all these probabilities are independent, thus it will be better to rewrite the above using short form representation. Since among block probabilities of length 2 only 2 are independent, we can take only two of the above equations, and express all block probabilities occurring in them by their short form representation, using eq. (51). This reduces eq. (80) to

$$P_{n+1}(0) = 1 - P_n(0) + P_n(00),$$
$$P_{n+1}(00) = 1 - 2P_n(0) + P_n(00) + P_n(000).$$
Although much simpler, the above system of equations still cannot be iterated, because on the right hand side we have an extra variable \( P_n(000) \). To put it differently, one cannot reduce iterations of \( F \) to iterations of a finite-dimensional map (in this case, two-dimensional map).

Before we continue, let us remark that although the aforementioned reduction is not, in general, possible, one can, nevertheless, in some circumstances compute \((F^n \mu)([b])\) for some selected (typically short) blocks \( b \) and for some reasonably simple \( \mu \). Such calculations use entirely different approach, and typically they exploit features of a particular CA rule, thus they cannot be easily generalized. For example, when \( \mu \) is a Bernoulli measure, probabilities of blocks of length up to 3 have been computed for a number of binary cellular automata rules, using the method of preimage counting \([13, 16, 17, 18, 19]\). We will, however, not be concerned with these methods here. Instead, we will now turn our attention to approximate methods for computing \( F^n \mu \).

Since the reduction of iterations of \( F \) to iterations of finitely-dimensional map is, in general, impossible, we can try to perform this task in an approximate fashion. In the case of rule 14 discussed above, we could use use Bayesian approximation for this purpose,

\[
P_n(000) \approx \frac{P_n(00)P_n(0)}{P_n(0)}.
\]

Equations (81) would then become

\[
\begin{align*}
P_{n+1}(0) &= 1 - P_n(0) + \frac{P_n(00)^2}{P_n(0)}, \\
P_{n+1}(00) &= 1 - 2P_n(0) + P_n(00) + \frac{P_n(00)^2}{P_n(0)}.
\end{align*}
\]

The above is a formula for recursive iteration of a two-dimensional map, thus one could compute \( P_n(0) \) and \( P_n(00) \) for consecutive \( n = 1, 2 \ldots \) without referring to any other block probabilities, in stark contrast with eq. (81). This, in fact, is the main idea behind the local structure approximation which will be formally introduced in the next section.

### 6. Approximate orbits of measures

Given the difficulty of finding \( F^n \mu \), H. Gutowitz et. al. \([1, 20]\) developed a method of approximating orbits of \( F \), known as the local structure theory.

Following \([1]\), let us define the scramble operator of order \( k \), denoted by \( \Xi^{(k)} \), to be a map from \( \mathcal{M}_\sigma(X) \), the set of shift-invariant measures on \( X \), to the set of finite block measures of order \( k \), such that

\[
\Xi^{(k)} \mu = \tilde{\mu}^{(k)}.
\]

The sequence

\[
\left\{ \left( \Xi^{(k)} F \Xi^{(k)} \right)^n \mu \right\}_{n=0}^{\infty}
\]

(85)
will be called the local structure approximation of level \( k \) of the exact orbit \( \{ F^n \mu \}_{n=0}^{\infty} \). Note that all terms of this sequence are Markov measures, thus the entire local structure approximation of the orbit lies in \( \mathfrak{M}^{(k)}(X) \).

The main hypothesis of the local structure theory is that eq. (85) approximates the actual orbit \( \{ F^n \mu \}_{n=0}^{\infty} \) increasingly well as \( k \) increases. The meaning of “approximates” is not rigorously defined in the original paper of H. Gutowit et. al. [1]. We will shortly prove that every point of the approximate orbit weakly converges to the corresponding point of the exact orbit as \( k \to \infty \). To do this, we need the following useful result.

**Proposition 6.1** Let \( k \) be a positive integer and \( b \in \mathcal{A}^* \). If \( k \geq |b| + 2r \), then

\[
F \mu([b]) = F \Xi^{(k)} \mu([b]) = \Xi^{(k)} F \mu([b]).
\]

To prove it, note that \( \mu([a]) = \tilde{\mu}^{(k)}([a]) \) for all blocks \( a \) of length up to \( k \). The first equality of the proposition can be written as

\[
\sum_{a \in \mathcal{A}^{|b|+2r}} w(a|b) \mu([a]) = \sum_{a \in \mathcal{A}^{|b|+2r}} w(a|b) \tilde{\mu}^{(k)}([a]). \tag{86}
\]

The equality holds when \( |a| \leq k \), that is, \( |b| + 2r \leq k \).

The second equality is a result of the fact that the scramble operator only modifies probabilities of blocks of length greater than \( k \). Since \( k \geq |b| + 2r \), we have \( |b| < k \) and therefore \( F \mu([b]) = \Xi^{(k)} F \mu([b]). \)

Since \( F^n \) can be considered as a cellular automaton rule of radius \( nr \), when \( k \geq |b| + 2nr \) we have \( F^n \mu([b]) = F^n \Xi^{(k)} \mu([b]) \). We can insert as many \( \Xi^{(k)} \) on the right hand side anywhere we want, and nothing will change, because \( \Xi^{(k)} \) does not modify relevant block probabilities. This yields an immediate corollary.

**Corollary 6.1** Let \( k \) and \( n \) be positive integers and \( b \in \mathcal{A}^* \). If \( k \geq |b| + 2nr \), then

\[
F^n \mu([b]) = \left( \Xi^{(k)} F \Xi^{(k)} \right)^n \mu([b]).
\]

This means that for a given \( n \), measures of cylinder sets in the approximate measure \( \left( \Xi^{(k)} F \Xi^{(k)} \right)^n \mu \) converge to measures of cylinder sets in \( F^n \mu \). By the virtue of Theorem 4.2 we thus obtain the following result.

**Theorem 6.1** Let \( F \) be a cellular automaton and \( \mu \) be a shift-invariant measure in \( \mathfrak{M}_\sigma(X) \). Let \( \nu^{(k)}_n \) be a local structure approximation of level \( k \) of the measure \( F^n \mu \), i.e., \( \nu^{(k)}_n = \left( \Xi^{(k)} F \Xi^{(k)} \right)^n \mu \). Then for any positive integer \( n \), \( \nu^{(k)}_n \Rightarrow F^n \mu \) as \( k \to \infty \).

7. Local structure maps

A nice feature of Markov maps is that they can be entirely described by specifying probabilities of a finite number of blocks. This makes construction of finite-dimensional maps generating approximate orbits possible.
If \( \nu_n^{(k)} = (\Xi^{(k)}F \Xi^{(k)})^n \mu \), then \( \nu_n^{(k)} \) satisfies recurrence equation

\[
\nu_{n+1}^{(k)} = \Xi^{(k)}F \Xi^{(k)}\nu_n^{(k)}.
\]  

(87)

On both sides of this equation we have measures in \( \mathcal{M}^{(k)}(X) \), and these are completely determined by probabilities of blocks of length \( k \). If \( |b| = k \), we obtain

\[
\nu_{n+1}^{(k)}([b]) = \Xi^{(k)}F \Xi^{(k)}\nu_n^{(k)}([b]),
\]

(88)

and, since \( \Xi^{(k)} \) does not modify probabilities of blocks of length \( k \), this simplifies to

\[
\nu_{n+1}^{(k)}([b]) = F \Xi^{(k)}\nu_n^{(k)}([b]).
\]

(89)

By the definition of \( F \),

\[
\nu_{n+1}^{(k)}([b]) = \sum_{a \in \mathcal{A}^{[b]}+2r} w(a|b) \left( \Xi^{(k)}\nu_n^{(k)} \right)([a]),
\]

(90)

and, by the definition of Bayesian approximation,

\[
\nu_{n+1}^{(k)}([b]) = \sum_{a \in \mathcal{A}^{[b]}+2r} w(a|b) \frac{\prod_{i=1}^{2r+1} \nu_n^{(k)}([a_{i,i+k-1}])}{\prod_{i=1}^{2r} \nu_n^{(k)}([a_{i+1,i+k-1}])}.
\]

(91)

To simplify the notation, let us define \( Q_n(c) = \nu_n^{(k)}([c]) \). Then, using consistency conditions in order to obtain on the right hand side expression involving only probabilities of blocks of length \( k \), we rewrite the previous equation to take the form

\[
Q_{n+1}(b) = \sum_{a \in \mathcal{A}^{[b]}+2r} w(a|b) \frac{\prod_{i=1}^{2r+1} Q_n(a_{i,i+k-1})}{\prod_{i=1}^{2r} \sum_{c \in \mathcal{A}} Q_n(ca_{i+1,i+k-1})}.
\]

(92)

The above equation can be written separately for all \( b \in \mathcal{A}^k \). If we arrange \( Q_n(b) \) for all \( b \in \mathcal{A}^k \) in lexicographical order to form a vector \( Q_n \), we will obtain

\[
Q_{n+1} = L^{(k)}(Q_n),
\]

(93)

where \( L^{(k)} : [0, 1]|\mathcal{A}|^k \to [0, 1]|\mathcal{A}|^k \) has components defined by eq. \( \text{[92]} \). \( L^{(k)} \) will be called local structure map of level \( k \). First \( N^k - N^{k-1} \) components of \( L^{(k)} \) will be denoted by \( L^{(k)}_{\text{Top}} \), and the remaining components by \( L^{(k)}_{\text{Bot}} \), and therefore the local structure map can be written as

\[
\begin{bmatrix}
Q^{(k)}_{\text{Top}} \\
Q^{(k)}_{\text{Bot}}
\end{bmatrix} \mapsto \begin{bmatrix}
L^{(k)}_{\text{Top}}(Q^{(k)}_{\text{Top}}, Q^{(k)}_{\text{Bot}}) \\
L^{(k)}_{\text{Bot}}(Q^{(k)}_{\text{Top}}, Q^{(k)}_{\text{Bot}})
\end{bmatrix}.
\]

(94)

By Proposition 3.2 \( Q^{(k)}_{\text{Bot}} \) can be expressed in terms of \( Q^{(k)}_{\text{Top}} \),

\[
Q^{(k)}_{\text{Bot}} = [0, \ldots, 0, 1]^T - (B^{(k)})^{-1} A^{(k)} Q^{(k)}_{\text{Top}},
\]

(95)
and, therefore, only the “top” component of our map needs to be considered,

$$Q^{(k)}_{Top} \mapsto L^{(k)}_{Top} \left( Q^{(k)}_{Top}, [0, \ldots, 0, 1]^T - (B^{(k)})^{-1} A^{(k)} Q^{(k)}_{Top} \right).$$  \hfill (96)

We will call the above map the reduced long form of the local structure map, and write it as

$$Q^{(k)}_{Top} \mapsto L^{(k)}_{red.long} \left( Q^{(k)}_{Top} \right).$$  \hfill (97)

Now using eq. (48), we have $Q^{(k)}_{Top} = M^{(k)}_{short} Q^{(k)}_{short}$, and we can change variables in eq. (96) from long to short block representation. This yields

$$Q^{(k)}_{short} \mapsto \left( M^{(k)}_{short} \right)^{-1} L^{(k)}_{red.long} \left( M^{(k)}_{short} Q^{(k)}_{Top} \right).$$  \hfill (98)

We will call the above map the reduced short form of local structure map, and write it as

$$Q^{(k)}_{short} \mapsto L^{(k)}_{red.short} \left( Q^{(k)}_{short} \right).$$  \hfill (99)

As an example, consider rule 184 given by

$$\begin{align*}
w(1|000) &= 0, \ w(1|001) = 0, \ w(1|010) = 0, \ w(1|011) = 1, \\
& \hspace{1cm} w(1|100) = 1, \ w(1|101) = 1, \ w(1|110) = 0, \ w(1|111) = 1,
\end{align*}$$

and suppose we wish to construct local structure map of level 2 for this rule. Let $P_n(b) = F^n \mu([b])$. Using eq. (76) we obtain for $r = 1$, $|b| = 3$

$$P_{n+1}(b) = \sum_{a \in A^5} w(a|b) P_n(a).$$  \hfill (101)

Using definition of $w(a|b)$ given in eq. (77) and transition probabilities given in eq. (100) we obtain

$$\begin{align*}
P_{n+1}(00) &= P_n(0000) + P_n(0001) + P_n(0010), \\
P_{n+1}(01) &= P_n(0011) + P_n(0100) + P_n(0101) + P_n(1100) + P_n(1101), \\
P_{n+1}(10) &= P_n(0110) + P_n(1000) + P_n(1001) + P_n(1010) + P_n(1110), \\
P_{n+1}(11) &= P_n(0111) + P_n(1011) + P_n(1111).
\end{align*}$$  \hfill (102)

This set of equations describes exact relationship between block probabilities at step $n+1$ and block probabilities at step $n$. Note that 3-block probabilities at step $n+1$ are given in terms of 5-blocks probabilities at step $n$, thus it is not possible to iterate these equations.

Local structure map of order 3, given by eq. (92), becomes

$$\begin{align*}
Q_{n+1}(00) &= \frac{Q_n(00)^3}{(Q_n(00) + Q_n(01))^2} + \frac{Q_n(00)^2 Q_n(01)}{(Q_n(00) + Q_n(01))^2} + \frac{Q_n(00) Q_n(01) Q_n(10)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))},
\end{align*}$$

24
\[Q_{n+1}(01) = \frac{Q_n(00)Q_n(01)Q_n(11)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}
+ \frac{Q_n(00)Q_n(01)Q_n(10)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}
+ \frac{Q_n(01)Q_n(11)Q_n(10)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}
+ \frac{Q_n(01)Q_n(11)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}.\]

\[Q_{n+1}(10) = \frac{Q_n(01)Q_n(11)Q_n(10)}{(Q_n(10) + Q_n(11))^2}
+ \frac{Q_n(10)Q_n(00)^2}{(Q_n(00) + Q_n(01))^2}
+ \frac{Q_n(00)Q_n(01)Q_n(10)}{(Q_n(00) + Q_n(01))^2}
+ \frac{Q_n(01)Q_n(10)^2}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}
+ \frac{Q_n(11)^2Q_n(10)}{(Q_n(10) + Q_n(11))^2}.\]

\[Q_{n+1}(11) = \frac{Q_n(01)Q_n(11)^2}{(Q_n(10) + Q_n(11))^2}
+ \frac{Q_n(01)Q_n(11)Q_n(10)}{(Q_n(00) + Q_n(01))(Q_n(10) + Q_n(11))}
+ \frac{Q_n(11)^3}{(Q_n(10) + Q_n(11))^2}.\]  (103)

Note that eq. (103) can be obtained from eq. (102) by replacing \(P\)'s by \(Q\)'s and expressing every 5-block probability by its Bayesian approximation of order 3.

According to Corollary 3.1 only first two components of \([Q_n(00), Q_n(01), Q_n(10), Q_n(11)]\) are independent, that is, \(Q_n(00), Q_n(01)\). This means that we can ignore last two equations in (103), making in the first two equations substitutions given by eq. (32), that is,

\[Q_n(10) = Q_n(01),\]  (104)
\[Q_n(11) = 1 - Q_n(00) - 2Q_n(01).\]  (105)

This yields reduced long form of the local structure map (cf. eq. 96),

\[Q_{n+1}(00) = \frac{Q_n(00)^2}{Q_n(00) + Q_n(01)} + \frac{Q_n(00)Q_n(01)^2}{(Q_n(00) + Q_n(01))(-Q_n(01) + 1 - Q_n(00))}.\]

\[Q_{n+1}(01) = Q_n(01)
\times \frac{(2Q_n(00)^2 - 2Q_n(00) + 4Q_n(00)Q_n(01) + Q_n(01)^2 - Q_n(01))}{(Q_n(00) + Q_n(01))(Q_n(01) - 1 + Q_n(00))}.\]  (106)
We now proceed to produce reduced short form of this map. In short block representation, we choose \( Q_n(0) \) and \( Q_n(00) \) as independent blocks, and probabilities of all other blocks of length 2 can be expressed by them,

\[
\begin{align*}
Q_n(01) &= Q_n(0) - Q_n(00), \\
Q_n(10) &= Q_n(0) - Q_n(00), \\
Q_n(11) &= Q_n(00) - 2Q_n(0) + 1.
\end{align*}
\]

With this change of variables, eq. (106) becomes

\[
\begin{align*}
Q_{n+1}(0) &= Q_n(0), \\
Q_{n+1}(00) &= \frac{Q_n(00)^2}{Q_n(0)} + \frac{Q_n(00)[Q_n(0) - Q_n(00)]^2}{Q_n(0)[1 - Q_n(0)].}
\end{align*}
\]

This is the reduced short form of the local structure map (cf. eq. 98). Note that this form is not only simpler than the original local structure map, but it also makes it easier to see an important property of the map, namely the fact that the probability of 0 is invariant. This actually is true for the orbit of rule 184: probability of 0 (and 1) stays the same along the orbit. We have here, therefore, an example of a case where the local structure map “inherits” a property of the rule it approximates. In this case, it inherits the so-called additive invariant.

Not only does the map inherit the invariant from the exact orbit of rule 184, but it also converges to the “right” value. One can easily find its fixed points, determine their stability, and from there determine \( \lim_{n \to \infty} Q_n(00) \). Since \( Q_n(0) \) is constant, let us denote \( Q_n(0) = 1 - \rho \), so that \( Q_n(1) = \rho \). Eqs. (107) then reduces to

\[
Q_{n+1}(00) = \frac{Q_n(00)^2}{1 - \rho} + \frac{Q_n(00)[Q_n(1 - \rho) - Q_n(00)]^2}{\rho(1 - \rho)}.
\]

This nonlinear difference equation has three fixed points, 0, \( 1 - \rho \) and \( 1 - 2\rho \). The second one, \( 1 - \rho \), is always unstable. The first one, 0, is unstable for \( \rho < 1/2 \), and stable for \( \rho > 1/2 \). The third one, \( 1 - 2\rho \), is is stable for \( \rho < 1/2 \), and unstable for \( \rho > 1/2 \). We can, therefore, write

\[
\lim_{n \to \infty} Q_n(00) = \begin{cases} 
1 - 2\rho, & \rho < 1/2 \\
0, & \rho \geq 1/2.
\end{cases}
\]

Remarkably, this agrees with the exact limiting value of \( P_n(00) = F^n \mu([00]) \) for rule 184 provided that \( \mu \) is a Bernoulli measure, as computed in [19]. Again, we can say that the local structure map in this case inherits the limiting value of the probability \( P_n(00) \) from the exact orbit.

8. Conclusions

We have formalized the idea of local structure theory and demonstrated that orbits of shift-invariant measures under probabilistic (or deterministic) CA can be approximated by orbits of \((N - 1)N^k\)-dimensional maps, called reduced local structure maps. The paper presented
detailed procedure for construction of such maps. After this foundation has been laid out, further research is clearly needed. The main question which remains is the relationship between orbits of reduced local structure maps and exact orbits. Theorem 6.1 reveals one such relationship, namely that points of the orbits of the local structure map weakly converge to corresponding points of the exact orbit. Much more, however, can be said. For example, as we already noticed in the case of rule 184, local structure map “inherits” an additive invariant form the exact orbit. One can prove that this is a general property which holds for arbitrary CA rule with additive invariant(s). Are other important properties of CA, such as, for example, nilpotency or equicontinuity, “inherited” in a similar fashion? Can we rigorously prove that certain features of exact orbits are preserved when exact orbits are replaced by local structure approximated orbits? What are these features? These questions are currently under investigation and will be reported in a follow-up paper.

9. Acknowledgements

The author acknowledges partial financial support from the Natural Sciences and Engineering Research Council of Canada (NSERC) in the form of Discovery Grant. Some calculations on which this work is based were made possible by the facilities of the Shared Hierarchical Academic Research Computing Network (SHARCNET:www.sharcnet.ca) and Compute/Calcul Canada.

References

[1] H. A. Gutowitz, J. D. Victor, and B. W. Knight, “Local structure theory for cellular automata,” Physica D 28 (1987) 18–48.

[2] P. Kůrka and A. Maass, “Limit sets of cellular automata associated to probability measures,” Journal of Statistical Physics 100 (2000) 1031–1047.

[3] P. Kůrka, “On the measure attractor of a cellular automaton,” Discrete and Continuous Dynamical Systems (2005) 524 – 535.

[4] M. Pivato, “Ergodic theory of cellular automata,” in Encyclopedia of Complexity and System Science, R. A. Meyers, ed. Springer, 2009.

[5] E. Formenti and P. Kůrka, “Dynamics of cellular automata in non-compact spaces,” in Encyclopedia of Complexity and System Science, R. A. Meyers, ed. Springer, 2009.

[6] S. Wolfram, “Statistical mechanics of cellular automata,” Reviews of Modern Physics 55 (1983), no. 3, 601–644.

[7] H. J. Brascamp, “Equilibrium states for a one dimensional lattice gas,” Communications In Mathematical Physics 21 (1971), no. 1, 56.

[8] M. Fannes and A. Verbeure, “On solvable models in classical lattice systems,” Commun. Math. Phys. 96 (1984) 115–124.

27
[9] M. Fréchet, “Sur l’intégrale d’une fonctionnelle étendue à un ensemble abstrait,” *Bulletin de la S. M. F.* **43** (1915) 248–265.

[10] A. Kolmogorov, *Grundbegriffe der Wahrscheinlichkeitsrechnung.* Springer-Verlag, Berlin, 1933.

[11] H. Hahn, “Über die Mutiplikation total-additiver Mengenfunktionen,” *Annali della Scuola Normale Superiore di Pisa* **2** (1933), no. 4, 429–452.

[12] K. R. Parthasarathy, *Introduction to Probability and Measure.* Springer-Verlag, New York, 1977.

[13] A. N. Kolmogorov and Y. V. Prohorov, “Zufällige funktionen und grenzverteilungssätze,” in *Bericht über die Tagung Wahrscheinlichkeitsrechnung und Mathematische Statistik*, pp. 113–126. Deutscher Verlag der Wissenschaften, Berlin, 1954.

[14] P. Bilingsley, *Convergence of Probability Measures.* John Wiley & Sons, New York, 1968.

[15] H. Fukś and J. Haroutunian, “Catalan numbers and power laws in cellular automaton rule 14,” *Journal of cellular automata* **4** (2009) 99–110.

[16] H. Fukś and A. Skelton, “Orbits of Bernoulli measure in asynchronous cellular automata,” *Dis. Math. Theor. Comp. Science* **AP** (2011) 95–112.

[17] H. Fukś and A. Skelton, “Response curves for cellular automata in one and two dimensions – an example of rigorous calculations,” *International Journal of Natural Computing Research* **1** (2010) 85–99, arXiv:1108.1987.

[18] H. Fukś, “Probabilistic initial value problem for cellular automaton rule 172,” *DMTCS proc.* **AL** (2010) 31–44, arXiv:1007.1026.

[19] H. Fukś, “Exact results for deterministic cellular automata traffic models,” *Phys. Rev. E* **60** (1999) 197–202, arXiv:comp-gas/9902001.

[20] H. A. Gutowitz and J. D. Victor, “Local structure theory in more than one dimension,” *Complex Systems* **1** (1987) 57–68.