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Exchange Processes with a Local Interaction: Invariant Bernoulli Measures

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Abstract. A general class of Markov processes with a local interaction is introduced, which includes exclusion and Kawasaki processes as a very particular case. Bernoulli invariant measures are found for this class of processes.

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1. Introduction

The goal of this paper is to introduce a class of processes with a local interaction which consists in the transformation of the internal degrees of freedom and/or chemical reactions. We call these processes *exchange* or *Boltzmann* processes as they model binary interactions of particles. The introduced class of processes includes such well-known processes as exclusion processes and Kawasaki processes.

The definition is as follows. Let G be a finite or countable graph with the set of vertices $V = V(G)$ and the set of edges $L = L(G)$. Let a set X be given, which can be interpreted as the set of all characteristics of a site $v \in V(G)$ and/or the set of all characteristics of the particles sitting at v (such as the types of particles, their form, energy etc.). We define *configuration* as a function x_v, $v \in V$, on the set of vertices with values in X.

On the set of configurations, X^V, a continuous time Markov process $\xi_t = \xi_t^{G,F,\{\lambda_l\}}$ is defined as follows. For each edge $l = (v, v') \in L(G)$, a transition occurs with the rate $\lambda_l = \lambda_l(x_v, x_{v'})$, independently of all other edges. For a given l, the transition is a simultaneous transformation (binary reaction) of the spins x_v and $x_{v'}$,

$$(x_v(t), x_{v'}(t)) \to (x_v(t+dt), x_{v'}(t+dt)) = F(x_v(t), x_{v'}(t)) \qquad (1.1)$$

where $F : S = X \times X \to S = X \times X$ is some fixed mapping. We always assume F to be symmetric, that is $Fj = jF$, where $j(x_1, x_2) = (x_2, x_1)$. This explains why the order of vertices in (1.1) is not important. Thus, the process on G is defined by a function F and by a set of symmetric functions $\lambda_l(x_v, x_{v'}) = \lambda_l(x_{v'}, x_v)$.

If the set X and graph G are finite, then this defines a finite continuous time Markov chain, which we denote by ξ_t. Otherwise, for the existence of the process, one should impose some weak restrictions on F and λ_l.

The introduced process is a process with a local interaction, which play nowadays an important role in constructing physical models, see for example [1–3]. A particular case are Kawasaki processes, where a pair of points exchanges spins, that is F is a permutation. Even more popular are exclusion processes where $X = \{0, 1\}$, and F is also a permutation. In general the choice of F should be determined by the transformation of degrees of freedom of neighbouring particles (for example of water molecules) or by chemical reactions. As far as we know, such processes were never studied in sufficient generality.

The first problem to be solved is as follows: for given F and λ_l, describe all invariant Bernoulli measures (IBM). A measure μ on X^V is called Bernoulli, if for some probability measure ν on X we have

$$\mu = \nu \times \nu \times \ldots = \nu^V.$$

Such measures are well-known and are very important for the study of exclusion processes, see [3]. In this paper, we give a description of invariant Bernoulli measures for given F.

2. Invariance criteria

We assume here that X and G are finite, and F is assumed to be one-to-one. Due to compactness, at least one invariant measure always exists. Moreover, if F is one-to-one, then the uniform measure on X^V is invariant. We want to know for which maps F there exist other invariant Bernoulli measures.

Let ν be a probability measure on X. Let us consider the measure $\nu^2 = \nu \times \nu$ on the set $S = X \times X$. Let ν^2 take k different values, $d_1, d_2, \ldots, d_k$. Define a partition $\{S_i\}$ of the set S such that S_i consists of all points of S where ν^2 takes the value d_i.

Note that the map F can be uniquely expanded on a finite number of cycles on S. Let $C_1, \ldots, C_n$ be the supports of these cycles.

Definition 2.1. We say that the measure ν *agrees with the map* F if the support of any cycle of F belongs to only one of the sets S_i, $i = 1, \ldots, k$. In other words, the partition $\{C_j\}$ is finer than the partition $\{S_i\}$: for any C_j there exists S_i such that $C_j \subseteqq S_i$.

The following result gives a convenient criterion to check whether a given Bernoulli measure is invariant for given F.

Theorem 2.1. *Assume that X and G are finite and F is one-to-one. Assume that for any edge l the rates $\lambda_l = \lambda_l(s)$ satisfy the condition: $\lambda_l(s) = \lambda_l(F^{-1}(s))$ for all $s \in S$. Then the following conditions are equivalent:*

1. *Bernoulli measure $\mu = \nu \times \nu \times \ldots = \nu^V$ is an invariant measure of the Markov process ξ_t for any finite graph G.*
2. *The measure ν^2 is an invariant measure of the Markov process ξ_t for the graph G_2 with two vertices and one edge between them.*
3. *The measure ν^2 is invariant with respect to F.*
4. *The measure ν agrees with F in the sense of Definition* 2.1.

Proof. Firstly, it is evident that conditions 3 and 4 are equivalent, that is, the invariance of ν^2 with respect to F is equivalent to the fact that ν^2 takes constant values on the support of each cycle of F. It is also evident that $1 \Rightarrow 2$.

Let us prove then that $2 \Rightarrow 1$. In fact, let G, X, F be given and let l be the edge with vertices v and v'. Denote $\xi_t^{(l)}$ the Markov chain on X^V having only transitions at the edge (v, v'),

$$(x_v, x_{v'}) \to F(x_v, x_{v'})$$

with the rates $\lambda_l(x_v, x_{v'})$, that is, the remaining $\lambda_{l'}(x_v, x_{v'}) = 0$, $l' \neq l$. It is clear that if the condition 2 holds, then the Bernoulli measure ν^V on G is invariant with respect to any Markov chain $\xi_t^{(l)}$. Then we get the assertion from the following general and evident proposition. Let a colection of Markov processes $\xi_t^{(l)}$ on the same state space A be given, with the rates $\lambda_{\alpha\beta}^{(l)}$, $\alpha, \beta \in A$, $\alpha \neq \beta$, correspondingly. Moreover, let all the processes have the same invariant measure $\pi = \{\pi_\alpha\}$. Then the Markov process on A with rates $\mu_{\alpha\beta} = \sum_l \lambda_{\alpha\beta}^{(l)}$, $\alpha \neq \beta$, has the same invariant measure. The proof of this proposition is immediately obtained by summing the equations for stationary probabilities of $\xi_t^{(l)}$ over l.

Let us prove now that $3 \Rightarrow 2$, that is, if $\nu^2(s) = \nu^2(F^{-1}(s))$ for any $s \in S$ then the measure ν^2 is an invariant measure of the Markov process ξ_t for the graph G_2 with two vertices and one edge between them. To do this, let us write down the equations for the stationary probabilities of the Markov chain on G_2:

$$\lambda_l(s)\nu^2(s) = \lambda_l(F^{-1}(s))\nu^2(F^{-1}(s)), \quad s \in S.$$

They evidently hold under our assumptions. It follows from this that condition 2 implies condition 3 as well. $\square$

3. Description of invariant measures

For given F, Theorem 2.1 allows to check whether a given Bernoulli measure ν^V is invariant or not. To classify all invariant measures ν for given F is a more complicated problem. We give now simple combinatorial algorithms which allow, for given F, to construct all IBM.

Let ν be a measure taking values $a_1, \dots, a_m$, all different. Denote $X_i = \{x : \nu(x) = a_i\}$ and $S_{ij} = (X_i \times X_j) \cup (X_j \times X_i) = S_{ji}$. We say that a measure ν is *a general situation measure* if all pairwise products $a_i a_j$ are different. The partition $X_1, \dots, X_m$ defines a $(m-1)$-parametric family $\{(a_1, \dots, a_m),\ a_1 + \dots + a_m = 1\}$ of general situation measures. We say that an IBM ν^V is a general situation measure if ν is a general situation measure. We will describe all such measures, under some assumptions. Let us note that for general situation measures any cycle C_k of F belongs to only one set S_{ij}, that is, all S_{ij} are different.

A set $A \subset S$ is called *connected*, if for any two elements $(a,b), (a',b') \in A$ there exists a chain of elements $(a_i, b_i) \in A$:

$$(a,b) = (a_1, b_1),\ (a_2, b_2),\ (a_3, b_3), \dots, (a_n, b_n) = (a', b')$$

in which all subsequent pairs have a common element, that is

$$(\{a_i\} \cup \{b_i\}) \cap (\{a_{i+1}\} \cup \{b_{i+1}\}) \neq \emptyset, \quad i = 1, \dots, n-1.$$

Obviously, any set B can be uniquely partitioned into connected components.

We are going to give an algorithm for constructing all general situation IBM in case when all cycles of F are connected.

Theorem 3.1. *If all cycles of F are connected then, among the partitions agreeing with F, there exists a unique minimal partition $\{S_{ij} = (X_i \times X_j) \cup (X_j \times X_i)\}$. Any general situation IBM belongs to the family of IBM defined by this minimal partition. The minimal partition $\{S_{ij}\}$ is constructed by the algorithm given in the proof of Lemma* 3.1

Definition 3.1. A set $A \subset S$ is called *half-admissible*, if it can be represented as $A = X_1 \times X_2$, where either $X_1 = X_2$ or $X_1 \cap X_2 = \emptyset$. A set $A \subset S$ is called *admissible*, if it can be represented as $A = (X_1 \times X_2) \cup (X_2 \times X_1)$, where either $X_1 = X_2$ or $X_1 \cap X_2 = \emptyset$.

Half-admissible and admissible sets are always connected.

Lemma 3.1. *For any connected set $B \subset S$, among admissible sets containing (covering) B there exists a unique minimal admissible set covering B.*

Proof. The proof of this lemma consists in direct construction of such covering set. Let us construct first a half-admissible set $X_1 \times X_2$ containing B. To do this, take some element $(a, b) \in B$. Put, for example, $a \in X_1, b \in X_2$. If $a = b$, then it follows that $X_1 = X_2$. In this case the minimal set will be the set $X_1 \times X_1$, where X_1 is the projection of B on X (the projection of the set $B \subset S = X \times X$ on X is the set of all elements $x \in X$ such that there exists $a \in X$ such that either (a, x) or (x, a) belongs to B).

Consider now the case when $a \neq b$. Then necessarily $b \in X_2$, and also for all $(a, x) \in B$ necessarily $x \in X_2$. Continuing this process, due to connectedness of B, we encounter all elements of B and will construct X_1 and X_2. During this process it can occur that some element c belongs both to X_1 and to X_2. Then, by definition of half-admissible set, it should be $X_1 = X_2$. The symmetrized set $\overline{B} = (X_1 \times X_2) \cup (X_2 \times X_1)$ is called the closure of the set B. The lemma is proved. □

Proof of Theorem 3.1. Let $\overline{C_i}$ be the closure of the cycle C_i. To each cycle C_i there corresponds a symmetric cycle C_i^{sym}, where all elements of C_i^{sym} are the permutations of the elements of C_i. Moreover, either $C_i^{sym} = C_i$ or $C_i^{sym} \cap C_i = \emptyset$. Then $D_i = \overline{C_i^{sym} \cup C_i}$ define a covering of the set S, however they can intersect with each other. If some D_1 and D_2 intersect, then their union is connected. In this case one can take $\overline{D_1 \cup D_2}, D_3, \ldots, D_m$ instead of the collection of sets $D_1, D_2, \ldots, D_m$. On each step of this procedure the number of sets in the covering diminishes by 1, and finally we get a system of non-intersecting admissible sets which defines the partition $\{X_i\}$, and thus all general situation IBM. The resulting partition does not depend on the order in which we choose the pairs of intersecting subsets, as at each step we take minimal admissible set. The theorem is proved. □

If there exist non-connected cycles, then several families of IBM are possible, as Example 3.3 shows. An algorithm for constructing all such families is similar, but more involved, we discuss it below.

Example 3.1. Let us consider Kawasaki processes, when F is the permutation. In this case all cycles have the length 1 or 2. Then each X_i consists of one point only, and each S_{ij} consists of one (if $i = j$) or two (if $i \neq j$) elements. Then any Bernoulli measure is invariant.

Example 3.2. Let $F(a, b) = (f(a), f(b))$, where f is a one-to-one mapping $X \to X$ having the cycles X_i. Then $S_{ij} = (X_i \times X_j) \cup (X_j \times X_i)$ define all IBM.

Example 3.3. The simplest example when there exist two general situation IBM is as follows. Let X consist of four points, that is $X = \{x_1, x_2, x_3, x_4\}$. Let any cycle of F consist of one point only, except for the flowing two cycles:

$$C_1 = \{(x_1, x_2), (x_3, x_4)\} \subset S$$

and the symmetric one,

$$C_1^{symm} = \{(x_2, x_1), (x_4, x_3)\},$$

consisting of two points. Then there are two admissible partitions, $X_1 = \{x_1, x_3\}, X_2 = \{x_2, x_4\}$ and $X_1' = \{x_1, x_4\}, X_2' = \{x_2, x_3\}$, which define two one-parametric families of general situation IBM.

Further on, we shortly describe the algorithm for constructing all families of IBM in the general case. Let us show first that for any set $B \subset S$ there exists a unique minimal covering (that is, the covering belonging to any such covering of the set B) by non-intersecting half-admissible sets. In fact, if B is not connected, then for any connected component B_i of B consider its closure $\overline{B_i}$. It is easy to see that $\overline{B_i}$ do not intersect. Then the minimal half-admissible sets covering them do not intersect as well.

Let C_i be all cycles of F, and C_{ij} be all connected components of the cycle C_i. Take the closure $\overline{C_{ij}}$ of each C_{ij}. Firstly, for any i we construct a minimal admissible set A_i containing all $\overline{C_{ij}}$. The problem is that there can be several such A_i (see Example 3.3). Then for given A_i we construct, as above, (already unique) minimal partition $\{S_{kl}\}$ such that each A_i belongs to one of the sets S_{kl}.

4. Generalizations and remarks

Maps which are not one-to-one

Let us consider the case when F is not one-to-one. A point $s \in S$ is called *cyclic* if $s = F^n(s)$ for some $n > 0$, where F^n is the nth iteration of the map F. The set of cyclic points is subdivided onto cycles. The remaining points are called *inessential*.

From the definition of invariant (with respect to F) measure it easily follows that the invariant measure is zero on the set of inessential points. Let a measure ν on X take values $a_0 = 0, a_1, \dots, a_k$. Put $X_i = \{x \in X : \nu(x) = a_i\}$, $X_0 \neq \emptyset$. Then $(X_0 \times X) \cup (X \times X_0)$ contains the set of inessential points and possibly also some cycles. Let $C_1, C_2, \dots, C_m$ be all the cycles of the map F which do not belong to $(X_0 \times X) \cup (X \times X_0)$.

If, instead of X, we consider the set $X \setminus X_0$, then $(X \setminus X_0) \times (X \setminus X_0)$ is invariant with respect to F, is a union of the cycles $C_1, C_2, \dots, C_m$, and moreover the map F on $(X \setminus X_0) \times (X \setminus X_0)$ is one-to-one. It means that the description of invariant measures can be reduced to the case when F is one-to-one.

Countable X

This case is quite similar to the case when X is finite. In fact, if F has infinite cycles, then ν^2 should be zero on them. Thus, one can delete from X

the projections of all infinite cycles, that is we can restrict ourselves to the case when all cycles are finite. All the rest is similar to the case of finite X.

Oriented graph

Our results take place also in more general case when the graph G is oriented. The map F from $S = X \times X$ to itself is not necessary symmetric. Moreover the intensities $\lambda_l(x_v, x_{v'})$ may be non-symmetric functions of the spin values. However, the condition $\lambda_l(x_v, x_{v'}) = \lambda_l(F^{-1}(x_v, x_{v'}))$ should be fullfilled.

Links with physics

The introduced processes have many links with physics, on the intuitive level. For example, the book [4] explains many facts of behaviour of liquids and amorphous bodies using stochastic exchange interaction between nearby molecules. It gives an alternative to the common approach based on hard-balls-type models.

However when one tries to derive an exchange process from the existing fundamental physical theory, one encounters many difficulties. For example, what is the set of states (that is the set X introduced above) for the water molecules? The simplest classical model of water molecule includes at least the lengths of segments OH and the angles between them. The known quantum mechanical model is even more complicated: it defines a tetrahedron using molecular orbitals [5]. Moreover, it is known that chemical bonds of hydrogenic character may appear between closely situated water molecules — one molecule can have up to 4 such bonds. They form a random graph of bonds (edges) which presumably defines such properties of water as density, viscosity, heat capacity etc., and their abnormal character comparing with other liquids. In this context one can remark that the time dependence, even random, $\lambda_l = \lambda_l(t)$ does not change the invariant measures, under keeping the symmetry condition for any t. This means also that the graph G itself (depending on the configuration of particles in the space) does not play an important role, as we can consider the complete graph where some $\lambda_l = 0$.

Some problems

It could be interesting to get similar results for the case when X is a smooth manifold. In this case conservation laws play an important role. In the frame of this paper, an additive conservation law is a function G on X such that if $F(x, y) = (x_1, y_1)$ then

$$G(x) + G(y) = G(x_1) + G(y_1).$$

If ν is an IBM and C is an arbitrary constant, then the conservation law is

$$G(x) = C \ln \nu(x).$$

Other interesting possibilities are when F is random (see some examples in [6]) or even when F is quantum and X is a Hilbert space.

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