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On the Inference of Deterministic Chaos: Evolutionary Algorithm and Metabolic P System Approaches

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***Abstract*—This paper shows the possibility of using Metabolic P systems (MP systems) for chaotic system identification-reconstruction and it compares presented results with previous ones obtained by evolutionary algorithms. An important potentiality of MP theory is given by its powerful computational chaos generation that can be also used as an internal module of evolutionary algorithms by increasing their ability in specific cases of their application. Reported numerical experiments are discussed at the end.**

I. Introduction

This paper shows the possibility of an alternative way for the analysis and generation of chaotic systems. In previous experiments it has been demonstrated that beside classical methods it is also possible to use evolutionary algorithms for this task [30]. It was shown that evolutionary algorithms are capable of the reconstruction of chaotic systems without any partial knowledge of the internal structure, i.e. based only on measured data. Five different evolutionary algorithms are presented in [30] and tested in two different sets of experiments. The system selected for numerical experiments was the well-known logistic map (1). For each algorithm, 100 repeated simulations were conducted for each set of experiments. According to obtained results it can be stated that evolutionary reconstruction is an alternative and a promising way to identify chaotic systems.

Also another, more classical and non-evolutionary approach for chaotic system reconstruction was presented in [3]. Such an approach is based on the design of unknown inputs multiple observers using Linear Matrix Inequalities (LMI) formulation. The objective is to estimate state variables of a multiple model subject to unknown inputs affecting both states and outputs of the system.

In this paper we introduce another alternative method for chaotic system identification-reconstruction based on Metabolic P systems (MP systems) [11]. The paper is organized as follows: in Section II the evolutionary identification of chaotic systems is shortly presented, by recalling some results recently achieved in the identification of the logistic map (1). In Section III MP systems are then introduced and finally applied to the problem of reconstructing chaotic systems in Section IV. At the end of the paper a conclusion section is also provided, which recalls the results presented in this contribution by indicating the main points of strength of the approaches herein described.

II. Evolutionary Identification of Chaotic Systems

An approach for reconstructing chaotic systems, entirely different from classical methods, is based on evolutionary algorithms. In [30] such algorithms have been applied on selected examples to test their capability to reconstruct chaotic systems. The well-known logistic map [28], [27], [23]

$$x \mapsto rx(1-x) \tag{1}$$

has been selected for experiments and the cost function has been designed so that its minimization should lead to the reconstruction of a system with the same behavior of (1). Four versions of SOMA [29], six versions of differential evolution [26], one version of genetic algorithm [7], simulated annealing [8], [2] and some evolutionary strategies [1] have been applied to identify the logistic map in a total of 1300 simulation cases. Among them, in [30] the original logistic map has been identified in 73 occasions (5.6% of the 1300 simulations) and similar systems that fit the behavior of the logistic map in 186 occasions (14.3%). Therefore, there was a total of 259 identified cases (19.92%). Best identifications of the logistic map are given in (2) - (8), while the identification of different structures that exhibit very close behavior (e.g. the same bifurcation diagram) are given in (9) - (12):

$$r(x-x^2), \tag{2}$$

$$x(r-rx), \tag{3}$$

$$rx-rx^2, \tag{4}$$

$$r(1-x)x, \tag{5}$$

$$-x(-r+rx), \tag{6}$$

$$x(1-x)r, \tag{7}$$

$$x^2(1/x-1)r, \tag{8}$$

$$x\left(r - rx + \frac{(1-r)\,x}{r^2\,(2r - x + rx)}\right), \tag{9}$$

$$x\left(r - rx + \frac{x^2}{r\left(\frac{1}{r} + r + \frac{r}{x} + rx\,(r+x)\right)}\right), \tag{10}$$

$$\frac{r(1-x)x(x + (-r+x)(r+x))}{-r^2 - x}, \tag{11}$$

$$x\left(r - \frac{r^3 x}{r + r^2 + x} - \frac{r^2 - 2r(r-x)}{-\frac{r^2}{x} + 2x}\right). \tag{12}$$

As a comparative method to evolutionary algorithms, we would like to introduce here a method based on Metabolic P systems (MP systems) [11], which can be used mutually with evolutionary algorithms for the identification-reconstruction of black-box dynamical systems.

III. Introduction to MP systems

Metabolic P systems (MP systems), based on Păun's P systems [24], [25], were introduced in [12], [9] for modeling *metabolic systems* by means of suitable multiset rewriting grammars. An MP system is essentially given by: (i) an *MP grammar*, which provides the set of *variables* and *rules* specifying the system evolution; (ii) the *temporal interval* τ of the dynamics discretization; (iii) the conventional *mole size* ν of variable quantities [11]. In the following systems the values of τ and ν are always unitary. Each rule of an MP grammar is given by a couple *reaction/regulator*, as in the following example:

$$\begin{array}{ll} r_1 : \emptyset \to A & \varphi_1 : 0.047 + 0.087 \cdot A \\ r_2 : A \to B & \varphi_2 : 0.002 \cdot A + 0.0002 \cdot A \cdot C \\ r_3 : A \to C & \varphi_3 : 0.002 \cdot A + 0.0002 \cdot A \cdot B \\ r_4 : B \to \emptyset & \varphi_4 : 0.04 \cdot B \\ r_5 : C \to \emptyset & \varphi_5 : 0.04 \cdot C. \end{array} \tag{13}$$

Reactions specify variable introduction/transformation/expulsion by means of a standard arrow notation. Regulators are instead formulae on the state of the system that permit to compute the speed of reactions at each step, by considering the temporal interval τ (therefore MP systems are deterministic and discrete systems).

In MP grammar (13) we have five rules over three variables (A, B and C). The first rule is an input rule, that is, it introduces quantity of type A in the system; rules 2 and 3 apply some transformations between variables and, finally, rules 4 and 5 expel quantities of type B and C from the system (output rules).

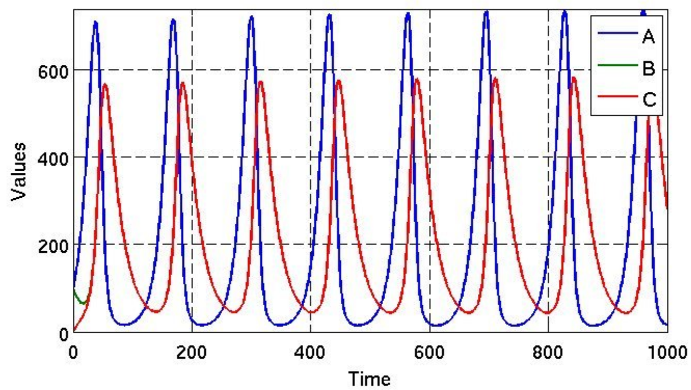

Fig. 1. The first 1000 steps of the dynamics of the MP system defined by MP grammar (13), computed by means of the EMA formula (14). The dynamics starts from initial values: $A[0] = 100$, $B[0] = 100$, and $C[0] = 0$.

Regulators permit the computation of the amounts that are consumed or produced by reactions at each simulation step. According to the type of the MP system, regulators are used during simulation according to different strategies (please refer to [11] for details). The most classical way of considering regulators is that defined in *MPF systems* (MP systems with fluxes), where regulators directly provide the fluxes of rules in the current state. In the following all the provided examples will be based on such kind of system. For example, by considering MP grammar (13), if at step i variable A has a value of $A[i] = 5$, then the flux $u_1[i]$ of rule r_1 at step i is computed by:

$$u_1[i] = 0.047 + 0.087 \cdot A[i] = 0.047 + 0.087 \cdot 5 = 0.482.$$

Therefore, in the next step the value of variable A will be increased by r_1 of this amount.

Let us assume to consider a system at some time steps $i = 0, 1, 2, \ldots$, with $i \in \mathbb{N}$. Let us also assume that a variable x is produced by rules r_1, r_3 and consumed by rule r_2. If $u_1[i], u_2[i], u_3[i]$ are the fluxes of the rules r_1, r_2, r_3, respectively, in the passage from step i (at time t) to step $i+1$ (at time $t+\tau$), then the variation $\Delta_x[i]$ of variable x at step i is given by:

$$\Delta_x[i] = x[i+1] - x[i] = u_1[i] - u_2[i] + u_3[i].$$

In MP systems, variables, reactions, and regulators specify the following discrete dynamics $(x[i] | i \in \mathbb{N})$ for any variable x, starting from a given value $x[0]$, called *Equational Metabolic Algorithm* (EMA):

$$\Delta_x[i] = x[i+1] - x[i] = \sum_{j=1}^{m} (\beta_j(x) - \alpha_j(x)) \cdot u_j[i] \tag{14}$$

where $r_j = \alpha_j \to \beta_j$ for $j = 1, \ldots, m$ are the rules, α_j, β_j are multisets, of reactants and products respectively, and $\alpha_j(x)$, $\beta_j(x)$ denote the multiplicity of variable x in α_j, β_j, respectively. In the following, the MP dynamics we will

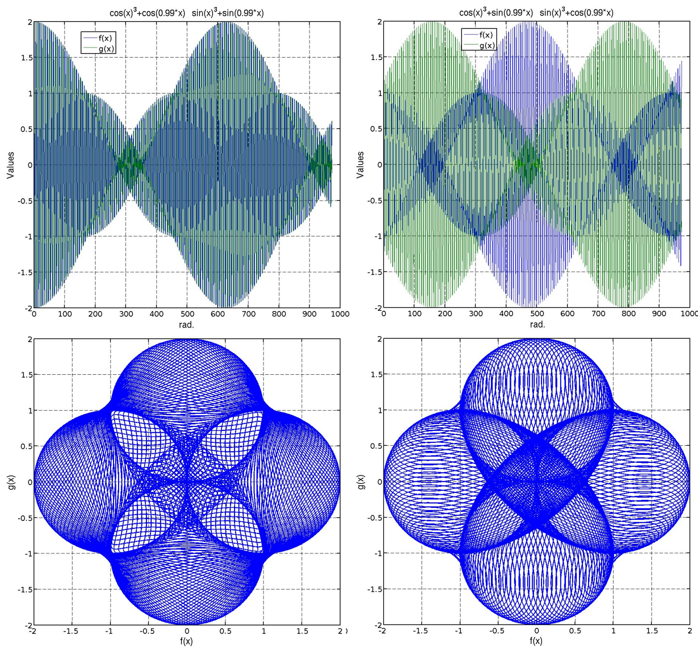

Fig. 2. Examples of complicated oscillators that can be obtained with simple MP grammars with linear regulators (see [15] for details).

present are computed in MATLAB[1] by applying the EMA formula given in (14). The first 1000 steps of the dynamics of the MP system defined by MP grammar (13) is depicted in Fig. 1.

The dynamics which can be modeled by MP systems can be very complicated even by considering simple MP grammars (i.e. with few variables and linear regulators). In [15] MP systems were successfully applied to the field of real periodical function approximation. In that work, we presented some interesting MP oscillators which are obtained by approximating the plot of some given periodical functions[2]. In Fig. 2 the dynamics of two MP oscillators are depicted, which have been computed by means of an MP grammar with only six variables and linear regulators.

The results obtained in [15] suggested some possible applications to specific cases of interest. In particular, the procedure introduced to define the models has been widely extended in [16], [17], [18] for defining *LGSS (Log–Gain Stoichiometric Stepwise Regression)*, a regression algorithm which derives MP models from the time series of observed dynamics.

LGSS provides a solution, in terms of MP systems, of the *dynamics inverse problem (DIP)*, that is, of the identification of (discrete) mathematical models exhibiting an observed dynamics and satisfying all the constraints required by the specific knowledge about the modeled phenomenon. The LGSS algorithm combines and extends the log–gain principles developed in the MP system theory [11] with the classical method of Stepwise Regression [6], which is a statistical regression technique based on Least Squares Approximation and statistical F–tests [4].

[1]See `http://www.mathworks.it/index.html` for details on the MATLAB software.

[2]The approximation order ranges from 10^{-6} to 10^{-14}, depending on the considered model.

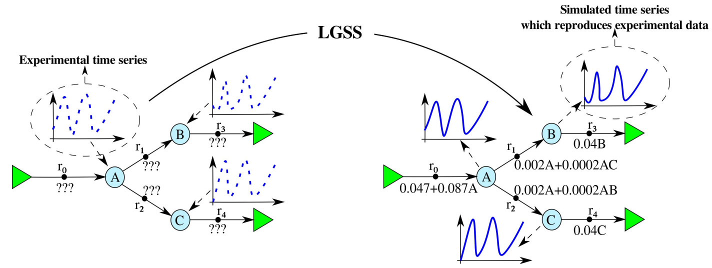

Fig. 3. The approach implemented by LGSS for the inference of MP models. The algorithm automatically computes regulator formulae for each reaction of the system starting from time series of variable observations and a set of basic functions (called regressors) that are used to compute regulators as linear combination of some of them. In this example, regulators have been inferred by considering as regressors all the monomials of A, B, and C of first, second and third degree (A, B, C, A^2, B^2, C^2, AB, AC, BC, A^3, B^3, C^3, A^2B, A^2C, B^2C, AB^2, AC^2, BC^2, ABC).

LGSS has been initially implemented in 2010 as a set of MATLAB functions and it is now part of a new Java library that will be soon distributed as open–source project. In order to start, LGSS requires the stoichiometry of the system (i.e. the set of reactions), the time series of observed variables, and, finally, a set of basic functions, called *regressors*, that will be used to infer regulators as linear combination of some of them.

It is important to stress that LGSS not only finds optimal values of system parameters, but *it suggests also the form of regulators* as a linear combination of basic functions among those specified by the user. This possibility could be very important in the case where the knowledge about the phenomenon under investigation is so poor that no clear idea is available about the kind of model underlying the observed behavior (see Fig. 3). Successful modeling results comprise metabolic dynamics, gene expression networks, and population dynamics [22], [21], [19], [15], [14], [20], [13].

IV. MP CHAOTIC SYSTEMS

In this section we will discuss some hints about the relationship between chaotic systems and MP systems. As introduced in the previous section, MP systems are essentially deterministic discrete systems which can be translated, by means of the EMA equation (14), as a suitable system of difference equations. In such systems, regulators play a role that is analogous to that played by derivatives in ODE systems. Despite these analogies, MP systems proved to be advantageous in many modeling situations which ranged from the theoretical field of real function approximation [15] to the modeling of complicated biological dynamics relevant in Systems Biology [22], [21], [19], [15], [14], [20].

From what emerged in our work, one of the big advantages of MP systems is related to the rule–based view of systems realized by MP grammars. In fact, such perspective is often more intuitive and closer to the logic of the phenomenon under examination than that provided by equations. Interestingly, this fact emerged in all the modeling fields approached with the MP theory, even the ones that are more theoretical and less related to biology. Encouraged by these considerations, we recently started a new line of investigation aiming at the definition of grammatical schemata that lead the system to reach a chaotic dynamics, under suitable conditions.

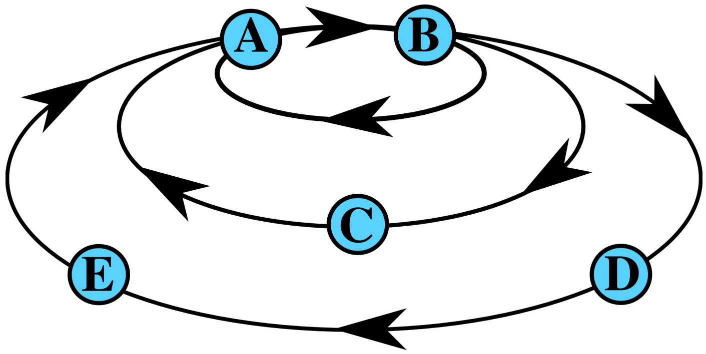

Fig. 4. The abstract schema of three overlapping transformation cycles (see also MP grammar (15)). Variable B is divided into three transformation cycles that cause the appearance of quantities of type A after a delay of 1, 2, or 3 simulation steps.

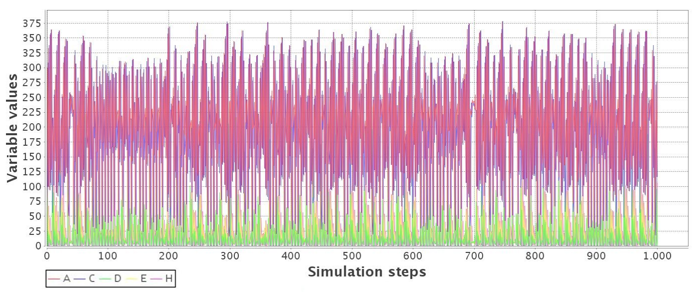

Fig. 5. The first 1000 steps of the dynamics of the MP system defined by MP grammar (15), computed by means of the EMA formula (14). The dynamics starts from initial values: $A[0] = B[0] = C[0] = D[0] = E[0] = 100$.

From our initial results emerged that grammatical schemata based on *overlapping transformation cycles* permit to reach quite easily chaotic dynamics. Fig. 4 provides an abstract schema of the concept of overlapping transformation cycles. The intuition behind this schema, which leads to a chaotic behavior, relies on the fact that the “matter” is continuously mixed up between transformation cycles of different length. The idea comes from [10], where it was introduced in the study of complex MP oscillators. The following MP grammar:

$$\begin{array}{ll} r_1 : A \rightarrow B & \varphi_1 : A \\ r_2 : B \rightarrow A & \varphi_2 : \frac{BC^2}{1.5+C^2} \\ r_3 : B \rightarrow C & \varphi_3 : \frac{B^2}{300+200C^2+B} \\ r_4 : B \rightarrow D & \varphi_4 : \frac{B}{1.5+C^2} \\ r_5 : C \rightarrow A & \varphi_5 : C \\ r_6 : D \rightarrow E & \varphi_6 : D \\ r_7 : E \rightarrow A & \varphi_7 : E \end{array} \tag{15}$$

is based on the abstract schema of Fig. 4. The dynamics of the MP system based on this grammar is depicted in Fig. 5. The behavior of all the variables of such system exhibits a chaotic pattern. In fact, the score computed by means of the 0–1 test [5], by considering the first 1000 steps of the time series of each one of the variable of the system, has been in all cases greater than 0.99 (the test returns a score close to 0 for non chaotic patterns and close to 1 for chaotic behaviors).

The importance of overlapping transformation cycles in MP grammar (15) is emphasized by the fact that the only non linear regulators are those of the rules having as reactant the variable B. In fact, these rules are those responsible of the its distribution between cycles. All the other rules implement delays of different length and are all linearly regulated.

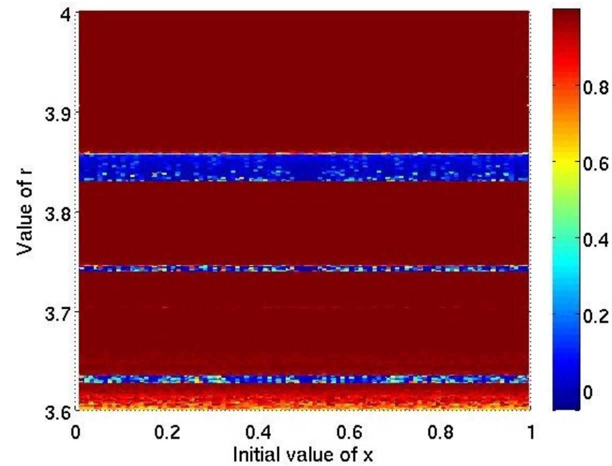

Fig. 6. Mosaic map which represents the value of the score computed by means of the 0–1 test [5], by considering the first 1000 steps of the time series generated by the logistic map, according to the considered initial value of x and the value of the parameter r. The most of the map is red (score near 1) indicating that the behavior generated by the map is chaotic. Blue areas represent *islands of stability* that arise for some isolated ranges of r.

A. Relationship between the logistic map and MP models based on overlapping transformation cycles

The logistic map is a polynomial mapping of second degree often cited as an archetypal example of how complex, chaotic behavior can arise from very simple non-linear dynamical equations [28], [27], [23]. According to (1), the logistic map is defined as:

$$x[i+1] = rx[i](1 - x[i]), \tag{16}$$

where x is a variable having a value between zero and one and r is a positive parameter. It is well known in literature that, regardless of the initial value of x, the map provides a chaotic behavior for values of r that range between 3.57 and 4 (except for some isolated ranges of r called *islands of stability*, see the mosaic map depicted in Fig. 6).

In the following we will show that the chaotic behavior of the logistic map can be generated by MP models based on overlapping transformation cycles. To do this, we rewrite (16) in order to define the MP grammar related to the logistic map. According to what introduced in Section III, the value of the variation $\Delta_x[i]$ of variable x at step i is given by:

$$\Delta_x[i] = x[i+1] - x[i]. \tag{17}$$

Therefore, if we substitute (16) in (17), we obtain:

$$\Delta_x[i] = rx[i](1 - x[i]) - x[i] \tag{18}$$
$$\Delta_x[i] = rx[i] - rx^2[i] - x[i] \tag{19}$$
$$\Delta_x[i] = (r-1)x[i] - rx^2[i]. \tag{20}$$

Equation (20) indicates that variable x is increased in terms of $(r-1)x$ and decreased in terms of rx^2 at each simulation

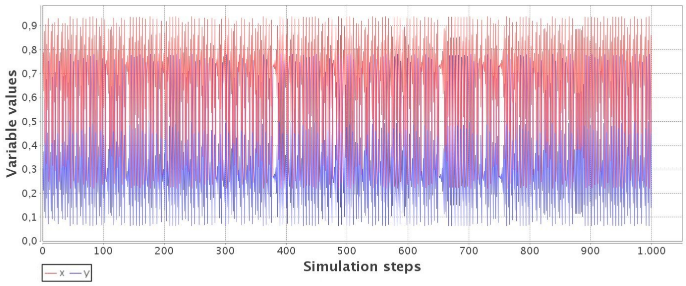

Fig. 7. The first 1000 steps of the dynamics of the MP system defined by MP grammar (22), computed by means of the EMA formula (14). The behavior generated is the same of a logistic map ($x[0] = 0.7$, $r = 3.75$). The behavior of variable y at each step i is such that $x[i] + y[i] = 1$.

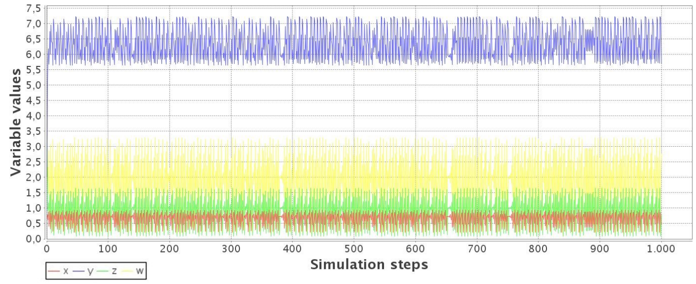

Fig. 8. The first 1000 steps of the dynamics of the MP system defined by MP grammar (26), computed by means of the EMA formula (14). The dynamics starts from initial values: $x[0] = 0.7$, $y[0] = 2.0$, $z[0] = 3.0$, and $w[0] = 4.0$.

step. This considerations can be translated to the following MP grammar:

$$\begin{array}{ll} r_1 : \emptyset \to x & \varphi_1 : (r-1)x \\ r_2 : x \to \emptyset & \varphi_2 : rx^2 \end{array} \tag{21}$$

that expresses in terms of input and output rules the variation of variable x. If we add to the system another variable y, initialized as $y[0] = 1 - x[0]$, then we can rewrite the grammar (21) in this way:

$$\begin{array}{ll} r_1 : y \to x & \varphi_1 : (r-1)x \\ r_2 : x \to y & \varphi_2 : rx^2 \end{array} \tag{22}$$

where input and output rules are replaced by transformations between x and y (see Fig. 7). This last grammar shows that the behavior of the logistic map can be generated by an MP grammar with one transformation cycle. Therefore the MP grammar (22), derived from the logistic map, constitutes the most simple MP model, generating a chaotic behavior, which is based on the concept of transformation cycles, as depicted in Fig. 4 (where only one transformation cycle is enough to obtain the chaotic behavior).

Starting from MP grammar (22) it is possible to define many other grammars exhibiting different chaotic behaviors by adding variables and reactions in order to increase the length or the number of overlapping transformation cycles in the system. The following MP grammars have been all derived from MP grammar (22):

- three variables, one transformation cycle:

$$\begin{array}{ll} r_1 : y \to x & \varphi_1 : (r-1)x \\ r_2 : x \to z & \varphi_2 : rx^2 \\ r_3 : z \to y & \varphi_3 : z \end{array} \tag{23}$$

- three variables, two overlapping transformation cycles:

$$\begin{array}{ll} r_1 : y \to x & \varphi_1 : rx \\ r_2 : x \to y & \varphi_2 : rx^2 \\ r_3 : x \to z & \varphi_3 : x \\ r_4 : z \to y & \varphi_4 : z \end{array} \tag{24}$$

- four variables, one transformation cycle:

$$\begin{array}{ll} r_1 : y \to x & \varphi_1 : (r-1)x \\ r_2 : x \to w & \varphi_2 : rx^2 \\ r_3 : w \to z & \varphi_3 : w \\ r_4 : z \to y & \varphi_4 : z \end{array} \tag{25}$$

- four variables, two overlapping transformation cycles:

$$\begin{array}{ll} r_1 : y \to x & \varphi_1 : (r-1)x \\ r_2 : x \to w & \varphi_2 : rx^2 \\ r_3 : w \to z & \varphi_3 : \frac{w}{2} \\ r_4 : w \to y & \varphi_4 : \frac{w}{2} \\ r_5 : z \to y & \varphi_5 : z \end{array} \tag{26}$$

All the MP grammars above provide chaotic behaviors (the score computed by means of the 0–1 test [5], by considering the first 1000 steps of the time series of each variable, has been in all cases greater than 0.99, see Fig. 8 for an example of dynamics).

B. *Inference of the logistic map by means of LGSS*

In previous sections we addressed the problem of defining deterministic chaotic systems by means of MP systems and we showed that the rule–based perspective of MP grammars provide important modeling advantages in the definition of such systems. In this section we would like to address the *inverse problem*, that is, we would like to start from a chaotic time series generated by a logistic map and then we would like to infer an MP grammar like the one in (21) that is able to generate that time series.

The possibility of inferring the logic behind a chaotic behavior is an interesting research area that grounds on the necessity of discerning between real noise and too complicated deterministic behaviors. The inference process will be computed by means of the regression algorithm LGSS, by providing as input the grammar

$$\begin{array}{ll} r_1 : \emptyset \to x & \varphi_1 : 0 \\ r_2 : x \to \emptyset & \varphi_2 : 0, \end{array} \tag{27}$$

a time series for x (that has been generated by a logistic map using a specific value of $x[0]$ and r) and a set of regressors for inferring regulators that comprehend the constant and monomials of x of first, second and third degree (x, x^2, x^3).

Even if the regression model seems to be quite simple, the inference process is not trivial because regressors are inserted in regulator formulae according to a stepwise approach based on least squares approximation and statistical partial F–tests [4]. The performance of such statistical tests, however, may be affected by the fact that the behavior we are trying to reconstruct is chaotic, and therefore hardly distinguishable from Gaussian noise.

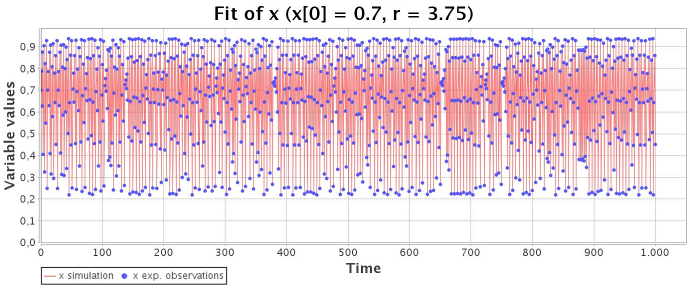

Fig. 9. The fit of an MP model inferred by LGSS approximating the chaotic behavior generated by a logistic map with $x[0] = 0.7$ and $r = 3.75$. Blue points give the chaotic behavior passed as input to LGSS, red line provides the simulation of the inferred model (1000 steps). The fit error is always of the same magnitude order of the precision accuracy reachable by the computer hosting the computation.

Despite this, in all the cases we considered LGSS has been able to reconstruct the MP grammar generating the chaotic profile by providing a very reliable estimate of the parameter r used for generating the input time series (the approximation error was in all the considered cases lower than 10^{-14}, which is the precision accuracy reachable by the computer hosting the computation). As a test we tried to reconstruct $40,000$ time series generated by means of a logistic map by considering initial values of x ranging between 0 and 1, and values of r ranging between 3.6 and 4.0. The high performance of LGSS made possible to complete all the regressions in less than ten minutes (on a standard laptop with a dual core CPU and 4 Gbyte of RAM memory, see Fig. 9 for an example of fit).

During the $40,000$ LGSS regressions we discovered also another important relationship between the values of $x[0]$ and r, used to generate a behavior by means of a logistic map, and the quantity of information that is necessary to reconstruct that behavior. In fact, we discovered that the minimum length of the time series of x that is necessary to pass as input to LGSS in order to complete the regression process (with an approximation error of r lower than 10^{-14}) depends on both $x[0]$ and r. Fig. 10 displays this relationship as a mosaic map. The pattern that is possible to distinguish has been never observed before and it emphasizes the power of LGSS in deciphering the regulation logic which is behind an observed phenomenon. In fact, even if the quantity of information that is present in a time series generated by a logistic map depends mostly by the value of r regardless of the value used for $x[0]$ (as represented in Fig. 6), the quantity of information that is necessary to reconstruct a logistic behavior seems to depend on both r and $x[0]$ with the same importance. A future research work will better investigate this aspect.

V. Conclusion

In the previous sections we showed that MP theory is comparable with evolutionary algorithms and both are capable of model identification-reconstruction of chaotic systems. In this paper the MP approach has been applied to some examples and mainly to the logistic map (16). In particular, both direct and inverse problems of chaotic systems have been addressed. In Section IV we discussed the importance of the rule-based view of systems provided by MP grammars in driving the process of definition of new models exhibiting chaotic behavior. Such

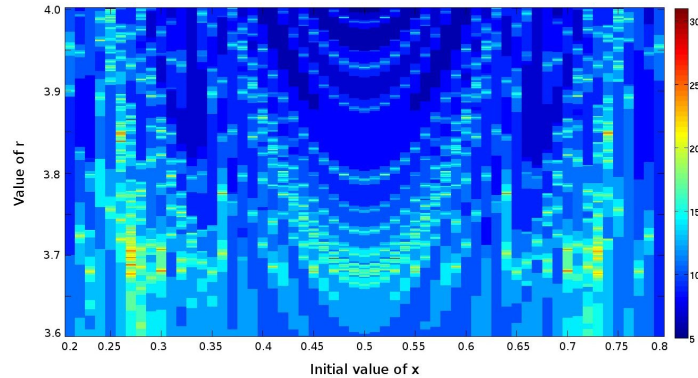

Fig. 10. Mosaic map which represents the minimum length of the x time series required by LGSS to complete the regression process (with an approximation error of r lower than 10^{-14}), according to the value of $x[0]$ and the value of the parameter r used for generating the behavior passed as input to the regression algorithm. In all the $40,000$ considered cases the minimum length of the required time series ranges between 5 and 31 points and varies according to the value of both $x[0]$ and r. The pattern that is possible to recognize shows that there is a relationship between the values of $x[0]$ and r used to generate a behavior by means of a logistic map and the quantity of information that is necessary to reconstruct that behavior.

a perspective permitted to introduce the abstract schema of overlapping transformation cycles that proved to be very useful for defining chaotic MP models. In Section IV-B, instead, we addressed the problem of inferring chaotic behaviors generated by the logistic map using the LGSS regression algorithm. In all the 40,000 regressions we did, we were able to reconstruct the original behavior by providing a very reliable approximation of the logistic parameter (approximation error lower than 10^{-14}). Moreover, we were also able to find a relationship between logistic parameters ($x[0]$ and r) and the quantity of information needed to reconstruct a logistic behavior. Such a relationship, represented in Figure 10 as a pattern of a mosaic map, has been never observed before and it emphasizes the power of LGSS in deciphering the regulation logic which is behind an observed phenomenon.

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