

Research paper

Generative complexity of Gray–Scott model

Andrew Adamatzky

University of the West of England, Bristol, United Kingdom



ARTICLE INFO

Article history:

Received 18 October 2016

Revised 26 July 2017

Accepted 22 August 2017

Available online 1 September 2017

ABSTRACT

In the Gray–Scott reaction–diffusion system one reactant is constantly fed in the system, another reactant is reproduced by consuming the supplied reactant and also converted to an inert product. The rate of feeding one reactant in the system and the rate of removing another reactant from the system determine configurations of concentration profiles: stripes, spots, waves. We calculate the generative complexity—a morphological complexity of concentration profiles grown from a point-wise perturbation of the medium—of the Gray–Scott system for a range of the feeding and removal rates. The morphological complexity is evaluated using Shannon entropy, Simpson diversity, approximation of Lempel–Ziv complexity, and expressivity (Shannon entropy divided by space-filling). We analyse behaviour of the systems with highest values of the generative morphological complexity and show that the Gray–Scott systems expressing highest levels of the complexity are composed of the wave-fragments (similar to wave-fragments in sub-excitable media) and travelling localisations (similar to quasi-dissipative solitons and gliders in Conway's Game of Life).

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1. Introduction

The Gray–Scott model [10,20,39] is a system of two reactants U and V : the reactant U is fed into the system, the reactants V is present in the system initially, one molecule of U reacts with two molecules of V producing three molecules of V . The model bears a striking similarity to the Lotka–Volterra model [24], where U is a prey, V is a predator and the Sel'kov model of glycolysis [42], where U is a substrate, V is a product; analogy with two-variable Oregonator model of Belousov–Zhabotinsky medium [15,38], where U is a catalyst and V is activator, are less obvious however spatio-temporal dynamics is often matching. The spatially extended Gray–Scott model with low coefficients of reactants diffusion shows a rich variety of concentration profile patterns: stripes, spots, waves [20,39]. Concentration patterns which attracted most attention include spots and auto-solitons [5,11,33,35,44], rings [29], self-replicating patterns [12,22,32,36,40], stripes [17,21], spiral waves [9]. The patterns are governed by a rate of feeding U and a rate of removal of V . Pearson [39] proposed a phenomenological classification of Gray–Scott model based of configurations of concentration profiles. The Pearson classification was detailed and extended by Munafa [30,31] and mapping between the Pearson–Munafa classes and Wolfram's classes of elementary cellular automata [46] has been proposed. Many interesting results have been obtained with Gray–Scott model but no evaluation of its complexity has been done so far.

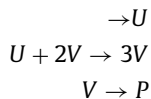
Complexity of reaction–diffusion (RD) systems is a weakly studied topic. We are aware of works publications where complexity is evaluated via entropy of a symbolic dynamics of RD equations and topology of attractors [48], rates of growth of small perturbations of solutions of reaction–diffusion equations [18], and from 'edge of chaos' perspective in analysing local

E-mail address: andrew.adamatzky@uwe.ac.uk

activity dynamics in cellular nonlinear networks [14]. The approach employed in [14] is adopted from cellular automata theory, namely entropy or mutual information measures proposed in [19,23] to classify cellular automaton rules quantitatively. Space-time dynamic of cellular automata gives a satisfactory yet very coarse-grained analogies of patterns exhibited in reaction–diffusion systems [6,8,45], even a binary-state two-dimensional automata exhibits most patterns found in Gray–Scott models [4], therefore that would be reasonable to apply complexity measures developed in cellular automata to the Gray–Scott system. Entropy has been applied to classify cellular automata for a long time [19,23], and it proved to be valid in supporting phenomenological classification of automaton dynamics and structures of their global transition graphs [47]. The compressibility [51] was proposed in [16] for classifying properties of patterns in spatially-extended non-linear systems, it was shown that the compressibility gives a finer discrimination on properties of the systems than Lyapunov exponent. Compression-based complexity of cellular automata evidence a match between the clusters of configuration compressibility and phenomenological classes of automaton behaviour [49]. Morphological richness (measured as a ratio of all possible configuration of a cell neighbourhood) and generative diversity (morphological complexity of a pattern developed from a single seed) [3] have been proved to be satisfactory tool for analysis of cellular-automaton evolution [34] and classification of excitation rules in two-dimensional cellular automata. Thus we evaluate morphological complexity of the Gray–Scott systems using Shannon entropy, Simpson diversity, and Lempel–Ziv compressibility. To avoid parameterisation of initial random conditions we considered only the generative complexity—the diversity of patterns developed from a point-wise local perturbation of otherwise resting medium. This approach is already proved to be efficient in studying complexity of cellular automata, and discrete models of excitable systems and populations [1–3].

2. Gray–Scott model

The Gray–Scott model [39] is comprised of two reactants U and V reacting as follows:



where P is inert product, reactant U is fed with rate k , reactant V is converted to inert product P with rate F , U reacts with V with rate 1. The corresponding reaction–diffusion equations for concentrations u and v are

$$\begin{aligned} \frac{\partial u}{\partial t} &= D_u \nabla^2 u - uv^2 + F(1 - u) \\ \frac{\partial v}{\partial t} &= D_v \nabla^2 v + uv^2 - (F + k)v \end{aligned}$$

We integrated the system using forward Euler method with five-node Laplace operator, time step 1 and diffusion coefficients $D_u = 2 \times 10^{-5}$ and $D_v = 10^{-5}$; these parameters have been chosen to stay compatible with [39]. We evaluated complexity measures by taking a grid of 256×256 nodes, each node x but four assigned concentration values $u_x = 1$ and $v_x = 0$, four neighbouring nodes at the centre of the lattice assigned $v_x = 1$: $\begin{array}{c|c} 1 & 1 \\ \hline 1 & 1 \end{array}$

For a given pair (k, F) the grid allowed to evolve until propagation of the perturbation, measured as $v > 0.3$, reached a boundary of the grid, or no changes between two subsequent concentration profiles observed, or a number of iterations exceeded 10^3 . The measures were calculated on concentration profiles after the halting. Snapshots illustrating the reaction–diffusion patterns are in RGB format. Concentrations of U and V in each node x are converted to RGB colour of the corresponding pixel x as $(R, G, B) = (u_x \cdot 255, 0, v_x \cdot 255)$. Scale 0.1 of original size.

3. Complexity measures

We evolved the systems and evaluated complexities for 8320 pairs (k, F) , where $k \in [0.020, 0.072]$, $F \in [0.010, 0.17]$, increments 0.001.

When evaluating complexity measures we binarised concentration profile of V as follows. The 256×256 nodes grid of concentrations is mapped onto an array L of 256×256 cells, where each cell x is assigned value ‘1’ if the concentration of V at the corresponding grid node x exceeds 0.3; otherwise the cell is assigned value ‘0’. Let $W = \{0, 1\}^9$ be a set of all possible configurations of a 9-node neighbourhood B_x including the central node x . Let B be a configuration of matrix L , we calculate a number of non-quiescent neighbourhood configurations as $\eta = \sum_{x \in L} \epsilon(x)$, where $\epsilon(x) = 0$ if for every resting x all its neighbours are resting, and $\epsilon(x) = 1$ otherwise.

The Shannon entropy H is calculated as $H = -\sum_{w \in W} (v(w)/\eta \cdot \ln(v(w)/\eta))$, where $v(w)$ is a number of times the neighbourhood configuration w is found in configuration B .

Simpson's diversity S is calculated as $S = \sum_{w \in W} (v(w)/\eta)^2$. Simpson diversity linearly correlates with Shannon entropy for $H < 3$; relationships become logarithmic for higher values of H (Fig. 1a).

Lempel–Ziv complexity (compressibility) LZ is evaluated by a size of concentration profiles saved as PNG files of the configurations, this is sufficient because the ‘deflation’ algorithm used in PNG lossless compression [7,13,41] is a variation of

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