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LETTER TO THE EDITOR

Invariants in automata networks

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Abstract. We give two extensions of Pomeau's additive invariant for reversible cellular automata and networks.

Introduced in the 1940s by McCulloch, Pitts, von Neumann and Ulam, automata networks have established themselves as unique tools for modelling computation, 'connectionist' and adaptive systems, and the emergence of complexity and organisation from the iteration of simple operations between simple elements (for recent reviews, see Bienenstock *et al* (1986) and Denker (1986)). Automata networks are nets of interconnected elements. Each element i has an internal state x_i (0 or 1) and interacts in discrete time steps with other elements j from some neighbourhood of i. In turn, it updates its own state according to an arbitrary preassigned 'rule', a Boolean function of the neighbourhood configurations at some past times:

$$x_i^t = f_i(\{x_j^{t-1}\}, \{x_j^{t-2}\}, \ldots, \{x_j^{t-k}\}). \tag{1}$$

As the present value x_i^t at site i depends on states from the previous k steps, the automaton defined by (1) is said to be of order k. The updatings in (1) are here understood to be *synchronous*: all the sites update their state simultaneously as a function of the non-updated values of the neighbours.

In the important special case of *cellular automata*, the variables are located on a *regular* array with *short-ranged* connections (the neighbourhood of i involves a small set of sites j close to i), and the law of evolution is uniform (f in (1) is the same at all sites i). These restrictions make cellular automata particularly well suited for the modelling of homogeneous physical systems with short-ranged microscopic interactions (Farmer *et al* 1984, Hayes 1984, Bennett *et al* 1986). Moreover, these restrictions have been exploited to advantage for the construction of machines that simulate cellular automata efficiently and that are modularly expandable (Toffoli 1984, Hillis 1985, Toffoli and Margolus 1985, Jenkins and Lee 1986). Though keeping these applications in mind, we shall not make use of these restrictions in the present discussion—the nets may be irregular and the neighbourhoods may be arbitrary.

This letter focuses on reversible automata, which are backward as well as forward deterministic: each configuration (or set of k successive configurations for systems of order k) admits a unique predecessor; the state space of the automata have no merging orbits. Reversible automata are of obvious physical interest: they can support realistic thermodynamics and hydrodynamics (Hardy *et al* 1976, Frisch *et al* 1986, Margolus *et al* 1986).

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Fredkin (see Margolus 1984, Vichniac 1984) has devised a simple way of constructing *reversible* second-order rules. Take any first-order rule A_i and subtract (modulo 2) from its value the state x_i^{t-2} that the considered site assumed at time $t-2$:

$$x_i^t = A_i(\{x_j^{t-1}\}) - x_i^{t-2} \qquad (\text{mod } 2). \tag{2}$$

This defines a second-order rule which is explicitly invertible, since (2) can be solved exactly for x_i^{t-2}, even if A_i itself is not invertible. Notice also that the subtraction modulo 2 is simply the exclusive OR Boolean operation.

A network with N sites will have N dynamical invariants, since the invertible evolution 'carries the memory' of the initial configuration. Of special interest are those invariants which are additive, i.e. which can be written as a sum over all sites i, in analogy with the additive canonical invariants of mechanics.

In an earlier letter, Pomeau (1984) constructs such an invariant for A_i of the form

$$A_i = \delta\left(\sum_{i,j} J_{i,j} x_j^{t-1}, q_i\right) \tag{3}$$

where the Kronecker δ is 1 if its two arguments are equal and 0 otherwise, and where the weights $J_{i,j}$ are assumed to be symmetric in i and j. In other words

$$x_i^t = \begin{cases} 1 - x_i^{t-2} & \text{if } \sum_{i,j} J_{i,j} x_j^{t-1} = q_i \\ x_i^{t-2} & \text{otherwise.} \end{cases} \tag{4}$$

Pomeau's invariant is defined as

$$\Phi^t = \langle x^t, Jx^{t-1}\rangle - \langle q, x^t - x^{t-1}\rangle \tag{5}$$

where x is the vector of components x_i, J is the matrix of elements $J_{i,j}$, and where the inner product notation implies a sum over all sites ($\langle u, v\rangle = \Sigma_i u_i v_i$).

Remarkably enough, Pomeau's invariant (5) takes precisely the form of a dissipative 'energy' which was introduced in the study of the length of transients and limit cycles in standard irreversible *first-order* neural networks (Goles 1983, see also Goles *et al* 1983, 1985).

In terms of spins $s_i = 2x_i - 1$ (such that $s_i = \pm 1$), the invariant takes the familiar form of an Ising energy

$$\Phi^t = \tfrac{1}{4}\sum_{i,j} J_{i,j} s_i^t s_j^{t-1} + \sum_i h_i(s_i^t + s_i^{t-1}) \tag{6}$$

with local external fields $h_i = \frac{1}{4}\Sigma_j J_{i,j} - q_i$, except that it involves spin values taken at two successive times. The invariant takes its simplest form

$$\Phi^t = \tfrac{1}{4}\sum_{i,j} s_i^t s_j^{t-1} \tag{7}$$

for the 'Q2R' cellular automaton (Vichniac 1984, 1986) defined by (4) with $q_i = 2$ at all sites of a two-dimensional square lattice with bonds $J_{i,j} = 1$ for i, j nearest neighbours, and vanishing otherwise. (In a D-dimensional lattice, one should use $q_i = D$.) In these simple cases we have two *non-interacting* Ising-type systems. If one of these systems is used to encode the immediate past of the other, Q2R provides an extremely efficient microcanonical algorithm for parallel simulations of the Ising model provided one replaces $t-2$ by $t-1$ in (4) and updates the lattice in a checkerboard pattern (Herrmann 1986). Q2R is capable of ergodicity breaking and also (Sorkin 1986) of an exceptionally large amount of ultrametricity, two important properties that characterise spin glasses.

Pomeau proposed the problem of extending (5) to the more general case where A_i admits several 'peaks':

$$A_i = \delta\left(\sum_{i,j} J_{i,j} x_j^{t-1}, q_i^{(1)}\right) + \ldots + \delta\left(\sum_{i,j} J_{i,j} x_j^{t-1}, q_i^{(s)}\right) \qquad (q_i^{(r)} \neq q_i^{(r')}). \quad (8)$$

If all the weights $J_{i,j}$ at a given i are equal, then A_i is a symmetric Boolean function, i.e. a function that is invariant under permutations of its arguments. First-order cellular automata based on such 'counting' functions are known to be capable of very complex behaviour (Toffoli 1977, Wolfram 1984, Vichniac 1984). The problem of constructing additive invariants for second-order automata with general counting A_i is thus expected to be very difficult. In this letter, we solve this problem in a special case and we construct invariants for a class of automata of higher order.

In the case where all the peaks in (8) belong to the same congruence class (mod p) for some integer p:

$$q_i^{(1)} = \ldots = q_i^{(s)} = Q_i \qquad (\text{mod}\, p) \quad (9)$$

the quantity

$$\Phi^t = \langle x^t, Jx^{t-1}\rangle - \langle Q, x^t + x^{t-1}\rangle \quad (10)$$

is an invariant of the evolution. All the operations in this definition are understood modulo p, including the summation implicit in the inner product. The invariance of Φ^t can be seen by calculating the difference

$$\Phi^t - \Phi^{t-1} = \langle Jx^{t-1} - Q, x^t - x^{t-2}\rangle \quad (11)$$

where again we assume that J is symmetric. The inner product vanishes term by term because at a site i either

$$\sum_{j=1}^{N} J_{i,j} x_j^{t-1} = Q_i \qquad (\text{mod}\, p) \quad (12)$$

or, when $A_i = 0$, x_i^t assumes the value x_i^{t-2}. The p values of Φ thus provide an invariant classification of the orbits. This classification is admittedly crude if p is small. However, the conserved quantity is of conspicuous physical interest because it is additive: it takes the form of a sum over sites of a 'local energy', and one can observe and study flows of Φ, especially if the coupling $J_{i,j}$ are short-ranged, as in cellular automata.

Our second extension of Pomeau's invariant deals with the single-peak case (3), but where the Fredkin construction (2) is extended to systems with k steps of memory:

$$x_i^t = \begin{cases} 1 - x_i^{t-k} & \text{if } A_i = 1 \\ x_i^{t-k} & \text{if } A_i = 0 \end{cases} \quad (13)$$

where A_i has a memory of order $k-1$:

$$A_i^t = \begin{cases} 1 & \text{if } \sum_{s=1}^{k-1} \sum_j J_{i,j}^s x_j^{t-s} = q_i \\ 0 & \text{otherwise.} \end{cases} \quad (14)$$

Rules of this type have been introduced by Caianiello in order to include hysteresis behaviour in the modelling of neural activity (Caianiello 1966). This transition rule, which defines the new value x_i^t of a site as a function of the past occupancies of its neighbourhood, now involves $k-1$ matrices $J^{(s)}$. We require that these matrices obey a 'palindrome condition':

$$J^{(k-s)} = \tilde{J}^{(s)} \qquad s = 1, \ldots, k-1 \tag{15}$$

where $\tilde{J}^{(s)}$ is the transpose of $J^{(s)}$. The corresponding invariant now takes the form

$$\Phi^t = \sum_{s=0}^{k-2} \left\langle x^{t-s}, \sum_{l=1}^{k-1-s} J^{(l)} x^{t-l-s} \right\rangle - \left\langle q, \sum_{s=0}^{k-1} x^{t-s} \right\rangle. \tag{16}$$

The invariance of Φ^t is also obtained here by constructing the difference:

$$\Phi^t - \Phi^{t-1} = \left\langle x^t, \sum_{l=1}^{k-1} J^{(l)} x^{t-l} \right\rangle - \left\langle x^{t-k}, \sum_{l=1}^{k-1} J^{(k-l)} x^{t-k} \right\rangle + \langle q, x^t - x^{t-k} \rangle. \tag{17}$$

The condition $J^{(k-l)} = \tilde{J}^{(l)}$ yields

$$\Phi^t - \Phi^{t-1} = \left\langle x^t - x^{t-x}, \sum_{l=1}^{k-1} J^{(l)} x^{t-l} - q \right\rangle. \tag{18}$$

Here again, the inner product vanishes term by term because, according to the evolution law (13) and (14), either

$$\sum_{l=1}^{k-1} \sum_{j=1}^{N} J_{i,j}^{(l)} x_j^{t-l} = q_i \tag{19}$$

or

$$x_i^t = x_i^{t-k}. \tag{20}$$

The invariance of Φ is thus established.

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