A Probabilistic Cellular Automaton Model for Developing Spatio-Temporal Patterns

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Abstract. A new approach of modeling for developing spatio-temporal patterns by using a probabilistic cellular automaton is proposed. The developing spatio-temporal patterns is too complicated to describe it by a small number of parameters. In our model, two states, i.e. black and white, are used to represent the state of cells. Therefore, the spatio-temporal pattern is treated as the developing black and white patterns. Our model has three model parameters that characterize the nearest neighbor interaction. These model parameters can detect the change of mechanism that generate patterns, which is one of the strong points of our model for monitoring the change of mechanism. Artificial black and white patterns are generated for a given parameters, and then the optimal parameters of the probabilistic cellular automaton model are sought. Optimization of the parameters is carried out by using two genetic algorithms: classical one and more sophisticated one. The convergence of the model parameters by two genetic algorithms is discussed. The fitness between the model and the observation is measured based on the Kullback-Leibler information.

1. Introduction

Pattern formation is one of the most interesting topics in nonlinear science. There are various patterns that are observed in nature (MANDELBROT, 1982; FEDER, 1988; VICSEK, 1989). However, to characterize the patterns is usually very difficult since almost all patterns in nature are very complicated. Furthermore, even for a static patterns it is not easy to characterize quantitatively, but some patterns dynamically change.

To characterize dynamically developing patterns, i.e. spatio-temporal patterns, is an exciting topic in various fields. Spatio-temporal patterns include too much information to characterize. Therefore, we focus on a black and white pattern. Black and white patterns are not special patterns. A lot of black and white patterns, e.g. mineral dendrite, are observed in nature (FEDER, 1988). In general, spatio-temporal patterns can be treated as

developing black and white pattern by carrying out the coarse-graining operation in timespace dimensions (HIRATA *et al.*, 2000a). For examples, a complex spatio-temporal seismic activity patterns are treated as developing black and white patterns (HIRATA and IMOTO, 1997; POSADAS *et al.*, 2000).

Developing black and white patterns is still complicated to describe by a small number of parameters. A cellular automaton is one of the tools of modeling for complex phenomena (FARMER *et al.*, 1984; TOFFOLI and MARGOLUS, 1987; ADAMATZKY, 1994). From the viewpoint of the interaction, we try to characterize developing black and white patterns by the nearest neighbor interaction that are described by a small number of parameters (HIRATA *et al.*, 2000a). In our approach, spatio-temporal patterns are reproduced by a probabilistic cellular automaton in which the nearest neighbor interaction are described by automaton rules. Our approach that describe the interaction has a merit that we get an information about the mechanism of pattern formation simultaneously.

2. A Probabilistic Cellular Automaton Model

Let us consider a probabilistic cellular automaton model in which the developing black and white patterns are described by only the nearest neighbor interaction. The spatiotemporal patterns are discretized in time, space and state dimensions. A square lattice is used as two-dimensional space, and the time step t_n is introduced by discretization in time space. The state of the cell (i, j) at the time step t_{n+1} , $s_{i,j}^{t_{n+1}}$, is determined by the state of the cell, $s_{i,j}^{t_n}$, and its nearest neighbor cells, $s_{i\pm 1,j\pm 1}^{t_n}$, at the time step t_n . Here, the state of the cells have only 2 available states (black and white), which is a discretization in states. The states of black and white are assigned 1 and 0, respectively. As a model dynamics, the evolution of the cell is described by the transition probability. Therefore, we obtain the following transition probability,

$$\operatorname{Prob}(s_{i,j}^{t_{n+1}} = 1) = f(s_{i,j}^{t_n}, s_{i\pm 1,j\pm 1}^{t_n})$$

$$\operatorname{Prob}(s_{i,j}^{t_{n+1}} = 0) = 1 - f(s_{i,j}^{t_n}, s_{i\pm 1,j\pm 1}^{t_n}).$$

$$(1)$$

Here, $\operatorname{Prob}(s_{i,j}^{t_{n+1}} = 1)$ is the probability that the state of the cell (i, j) will be 1 at t_{n+1} . As the value of the state, 0 or 1, is not essential, we can assign -1 or 1 to the states like as Ising model. Our model is applicable to the complicated spatio-temporal patterns, such as spatio-temporal seismic activity patterns. As for application of the model to the seismic activity patterns, we may use that state of cells is active (1: black) or inactive (0: white) (HIRATA and IMOTO, 1997; POSADAS *et al.*, 2000).

A probabilistic cellular automaton model for developing black and white patterns is shown in Fig. 1. The model has three parameters (p_1, p_2, p_3) that characterize the nearest neighbor interaction. In this model, only nearest neighbor interaction is considered so that the small template shown in Fig. 1 is used. Let us consider the meaning of the model shown in Fig. 1. In case of its four nearest neighbor cells being the states of 0 (white), the



Fig. 1. A probabilistic cellular automaton model.

probability of the cell with the state of 1 (black) at time step t_n being the state of 1 at t_{n+1} is p_1 . The cells with the state of 1 increases the probability of the nearest neighbor cell becoming the state of 1 by p_2 . In the case of $p_2 > 0$, the effect is activation and in the case of $p_2 < 0$, the effect is inhibition. The transition probability (in other word, the conditional probability) of the cell is a function of the cell and its nearest neighbor cells' states. When the number of nearest neighbor cells with the state of 1 is 4, 3, 2, or 1, the transition probability of the cell becoming black cell is increased by $4p_2$, $3p_2$, $2p_2$, or p_2 , respectively. If the cell's state is white, p_3 is used instead of p_1 . Therefore, we can rewrite Eq. (1), and obtain the transition probability as a function of n and $s_{i,j}^{t_n}$,

$$\operatorname{Prob}\left(s_{i,j}^{t_{n+1}}=1\right) = f\left(s_{i,j}^{t_n},n\right) = f\left(S_{i,j}^{t_n}\right).$$
(2)

Here, *n* is the number of nearest neighbor cells of which states are 1 (: black) at the time step t_n . For simplicity, we will use the notation of $S_{i,j}^{t_n}$ that represent the state of the (i, j) and number of its neighbor cells with state of 1. $(S_{i,j}^{t_n} = (s_{i,j}^{t_n}, n))$. In our model, the number of black nearest neighbor cells, *n*, is considered like as Ising model.

The meaning of parameters are summarized following:

The meaning of p_1 : If p_1 is large value, the probability that the cell of the state 1 at t_n will be in the state of 1 at t_{n+1} is high. The value of p_1 is non-negative $(0 \le p_1 \le 1)$.

The meaning of p_2 : The parameter p_2 describes the nearest neighbor interaction. In case of $p_2 > 0$, the effect of the interaction is excitation. In case of $p_2 < 0$, the effect of the interaction is suppression. T. HIRATA et al.



Fig. 2. Ten available states on the template that consist of the center cell and nearest neighbor cells and transition probabilities ($f(S_{l,i}^{(n)})$).

The meaning of p_3 : The meaning of p_3 is the background activity when the cell is in the state of 0 at t_n ($0 \le p_3 \le 1$).

Ten available state of $S_{i,j}^{t_n}$ are shown in Fig. 2. By using $S_{i,j}^{t_n}$ instead of $s_{i,j}^{t_n}$, $s_{i\pm 1,j\pm 1}^{t_n}$, the number of states considered are reduced from $2^5 = 32$ (black and white pattern on the small template) to 10 (HIRATA *et al.*, 2000b). According to the rules, transition probability Prob($s_{i,j}^{t_{n+1}} = 1$) is given by the function of $S_{i,j}^{t_n}$. The transition probability is shown at the bottom of the template in Fig. 2. There is a possibility that the transition probability calculated by the rule shown in Fig. 2 is larger than 1 for some parameter set of (p_1, p_2, p_3) . In such a case, the transition probability is assigned to 1.

3. Optimization of the Model by Genetic Algorithm

Our probabilistic cellular automaton model where nearest neighbor interaction is described by the parameter (p_1, p_2, p_3) can reproduce various patterns, e.g. random pattern, clustering pattern. Clustering patterns are often observed in nature (e.g., HIRATA and IMOTO, 1991) and attract scientists' attention (BAK *et al.*, 1987). The black and white pattern of Ising model at the critical temperature is one of the examples of clustering. In this case, p_2 will be positive value. The random black and white patterns are easily reproduced by the parameter set $(p_2 = 0)$ that means no interaction.

One of the most important part in the model is to find out the best fit parameter for given observational patterns. In this paper, we generate the artificial observational black and white patterns by using the parameter set (p_{1a}, p_{2a}, p_{3a}) . After that, we try to find out the best fit parameter set for artificial patterns by using the genetic algorithms.

3.1. Artificial black and white patterns

First, we produce the developing black and white patterns by Monte Carlo simulation at the given parameter set (p_{1a}, p_{2a}, p_{3a}) . In this study, we used the parameter set of (p_{1a}, p_{2a}, p_{3a}) .

Evolution of black and white patterns



Time

Fig. 3 An example of developing black and white patterns that generated by Monte Carlo simulations.

 p_{3a}) = (0.35, 0.15, 0.02) for Monte Carlo simulation. Then, we will seek the best model parameters by analyzing the patterns generated by the simulation.

Figure 3 is the developing black and white patterns obtained by Monte Carlo simulation. A 40 × 40 cells is used for generating an artificial developing black and white patterns. At the Monte Carlo simulation, one of the 40 × 40 cells is chosen at random and the state of the chosen cell is up to date at the probability according to the Eq. (2) (see Fig. 2). In Fig. 3, the patterns are shown every one Monte Carlo step. (As the number of the cells is 1600, the procedure in which one of the cells is randomly chosen and up to date is repeated by 1600 times in one Monte Carlo step. This means that one Monte Carlo step is equivalent to 1600 discrete time steps.) The periodical boundary conditions are used in Fig. 3. As an initial pattern, the random black and white pattern is used. To avoid the influence of the initial pattern, the evolving patterns after 1000 Monte Carlo steps are used, which are shown in Fig. 3. Since $p_{2a} = 0.15$ is positive, clustering patterns are observed in Fig. 3.

3.2. Genetic algorithms

Two kinds of genetic algorithms are used for finding out the optimal parameter sets.

• Classical genetic algorithm.

• Sophisticated genetic algorithm (crossover, elite strategy are added to classical one).

At first, we will describe algorithm of classical one. The procedure is following:

(1) Random 10 genes (parameter sets of (p_1, p_2, p_3) : p_1, p_2, p_3 are random values) are generated as initial values.

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(2) Mutations: The gene with the parameter of (p_1, p_2, p_3) is changed to one with the parameter of $(p_1 + \delta p_1, p_2 + \delta p_2, p_3 + \delta p_3)$. Here, $\delta p_1, \delta p_2, \delta p_3$ are small random values.

(3) Measurement of fitness of the genes: The fitness between model parameters and observational patterns are measured by Kullback-Leibler information.

(4) Natural selection: If the new gene by mutations gets better value than previous gene, the evolution occurs. Otherwise, the previous gene is used again (no evolution).

We calculate the procedure of (2)–(4) repeatedly. During these procedures, the genes will evolve to one that is the best fit for the environment (best fit for the observational data set).

In general, there is a bare possibility that the selected genes will fall into the local minimum state in optimization by using the genetic algorithm. However, this problem is avoidable by using a number of genes. Therefore, at least the best gene will not fall into the local minimum state if a number of genes, e.g. 10 genes in this study, are used.

The most important part in the above mentioned procedure is how to measure the fitness between the model and the observational pattern. The fitness of the model for the observational data can be measured by Kullback-Leibler information (SAKAMOTO *et al.*, 1986). The measurement of fitness by Kullback-Leibler information is based on the maximum log likelihood. In this study, therefore, the fitness is measured by Kullback-Leibler information. Kullback-Leibler information I is given by

$$I(p;q) = \sum P_i \log \frac{P_i}{Q_i}.$$
(3)

Here, P_i is true distribution (that is approximated by observational data), Q_i is the distribution obtained by the model, and Σ means summing up. The negative of Kullback-Leibler information, -I(p; q), is called the entropy. In this study, P_i , Q_i are probability distributions.

 $s_{i,j}^{t_{n+1}}$ is the future state of the (i, j) cell at the time step t_{n+1} . $S_{i,j}^{t_n}$ is the state of the (i, j) cell and its nearest neighbor cells at the time step t_n : There are 10 available states. $P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n})$ is a joint probability distribution. $P_{\text{model}}(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n})$ is a joint probability distribution calculated by the parameters of the model. Kullback-Leibler information is rewritten,

$$I(p;q) = \sum P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}) \log \frac{P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n})}{P_{\text{model}}(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n})}.$$
(4)

The $P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n})$ and $P(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})$ is related by the following multiplicative law,

$$P\left(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}\right) = P\left(s_{i,j}^{t_{n+1}} \middle| S_{i,j}^{t_n}\right) P\left(S_{i,j}^{t_n}\right).$$
(5)

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Here, $P(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})$ is a conditional probability distribution, and $P(S_{i,j}^{t_n})$ is probability of $S_{i,j}^{t_n}$ at t_n . Substituting Eq. (5) into Eq. (4), Kullback-Leibler information is given by

$$I(p;q) = \sum P\left(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}\right) \log \frac{P\left(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n}\right) P\left(S_{i,j}^{t_n}\right)}{P_{\text{model}}\left(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n}\right) P_{\text{model}}\left(S_{i,j}^{t_n}\right)}.$$
(6)

By using the following approximation $P(S_{i,j}^{t_n}) \approx P_{\text{model}}(S_{i,j}^{t_n})$, we obtain

$$I(p;q) \approx \sum P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}) \log \frac{P(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})}{P_{\text{model}}(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})}.$$
(7)

 $P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}), P(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})$ are obtained by counting the histogram of the observational data. Note that the Kullback-Leibler information, I(p; q), given by Eq. (7) may be less than 0 in some cases due to approximation $P(S_{i,j}^{t_n}) \approx P_{\text{model}}(S_{i,j}^{t_n})$, although the original Kullback-Leibler information defined by Eq. (3) should be larger than 0.

When (p_1, p_2, p_3) is given, we can calculate $P_{\text{model}}(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})$ according $P_{\text{model}}(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n}) = f(S_{i,j}^{t_n})$ shown in Fig. 2. The above described Kullback-Leibler information is used in natural selection. The optimum model parameters are those that minimize the value of Kullback-Leibler information.

The optimization is carried out by 10000 mutations. The evolution of one of 10 genes with parameters (p_1, p_2, p_3) and Kullback-Leibler information, *I*, are shown in Fig. 4. The initial values of ten genes are given by random number $(0 < p_1, p_3 < 1, -0.2 < p_2 < 0.2)$. In Fig. 4, the information, *I*, always decrease during evolution because the mutated gene can survive when fitness is improved. After about 400 mutations, the parameters converged. The evolution of 10 genes are shown in Fig. 5. After 500 mutations, all genes converge to the same values $(p_1, p_2, p_3) = (0.351, 0.143, 0.022)$ within the deviation of ± 0.001 .

The optimization of the parameter is carried out more sophisticated genetic algorithm. The sophisticated genetic algorithm is following:

(1) Random 10 genes (parameter sets of (p_1, p_2, p_3) : p_1, p_2, p_3 are random values) are generated as initial values.

(2) Mutations: The gene with the parameter of (p_1, p_2, p_3) is changed to one with the parameter of $(p_1 + \delta p_1, p_2 + \delta p_2, p_3 + \delta p_3)$. Here, $\delta p_1, \delta p_2, \delta p_3$ are small random values.

(3) Measurement of fitness of the genes: The fitness between model parameters and observational patterns are measured by Kullback-Leibler information.

(4) Natural selection: If the new gene by mutations gets better value than previous gene, the evolution occurs. Otherwise, the previous gene is used again (no evolution).

(5) Elite strategy: The worst gene is exchanged by a new gene $(p_1^{\text{best}}, p_2^{\text{second}}, p_3^{\text{best}})$ generated by crossover. Here, $(p_1^{\text{best}}, p_2^{\text{best}}, p_3^{\text{best}})$ is the parameter set of the best gene and $(p_1^{\text{second}}, p_2^{\text{second}}, p_3^{\text{second}})$ is the parameter set of the second best gene.



Fig. 4. Evolutions of the parameters and Kullback-Leibler information. Fig. 5. Evolutions of the parameters and Kullback-Leibler information for all genes.



Fig. 6. Same as Fig. 4 for the best gene by the sophisticated genetic algorithm. Fig. 7. Same as Fig. 4 for the worst gene by the sophisticated genetic algorithm.

We calculate the procedure of (2)–(5) repeatedly. The difference of sophisticated algorithm from classical one is an introduction of an elite strategy and crossover. The elite strategy is that the worst gene is replaced by the new gene generated by crossover.

The evolution of the parameters (p_1, p_2, p_3) and Kullback-Leibler information by the sophisticated genetic algorithm are shown in Fig. 6. In Fig. 6, the behavior of the best fit gene is shown. The rate of convergence by sophisticated algorithm is much faster than one by classical one. The behavior of worst gene is also shown in Fig. 7. Due to the elite strategy, the convergence is very quick. The parameters of the genes converges to $(p_1, p_2, p_3) = (0.350, 0.143, 0.023)$ that is almost same value obtained by classical algorithm. After about 200 mutations, the values of the parameters converged.

The information flow from the past states to the future states can be estimated by using mutual information. Mutual information $I(s_{i,j}^{t_{n+1}}; S_{i,j}^{t_n})$ is defined by

$$I\left(s_{i,j}^{t_{n+1}}; S_{i,j}^{t_n}\right) = \sum P\left(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}\right) \log_2 \frac{P\left(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}\right)}{P\left(s_{i,j}^{t_{n+1}}\right) P\left(S_{i,j}^{t_n}\right)}.$$
(8)

Here, $P(s_{i,j}^{t_{n+1}})$ is the probability of $s_{i,j}^{t_{n+1}}$ at t_{n+1} .

We can rewrite it as

$$I(s_{i,j}^{t_{n+1}}; S_{i,j}^{t_n}) = \sum P(s_{i,j}^{t_{n+1}}, S_{i,j}^{t_n}) \log_2 \frac{P(s_{i,j}^{t_{n+1}} | S_{i,j}^{t_n})}{P(s_{i,j}^{t_{n+1}})}$$
(9)

by using a multiplicative law. The mutual information give us the amount of information transmission from the past to the future. The value of the best model's entropy (the negative Kullback-Leibler information -I(p; q)), must be less than the mutual information (SHAW, 1984). Therefore, we cannot improve the model in order that the model's entropy will be beyond the mutual information. In our study, the mutual information is 0.2585 bit, and the maximum of the model's entropy is 0.233 bit.

4. Discussion

The spatio-temporal black and white patterns are reproduced by the probabilistic cellular automaton model from a given patterns. The model have three parameters (p_1, p_2, p_3) that characterize nearest neighbor interaction. By genetic algorithms, the optimization of the parameters were carried out. Both classical and sophisticated genetic algorithms can get very good optimal parameters. Results of optimization are following: Classical genetic algorithm: $(p_1, p_2, p_3) = (0.351, 0.143, 0.022) \pm 0.001$; Sophisticated genetic algorithm: $(p_1, p_2, p_3) = (0.350, 0.143, 0.023)$. Although the same optimum parameters were obtained by both algorithms, the convergence by sophisticated one is faster than classical one. Efficiency of sophisticated genetic algorithm is shown in this study.

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Our model is applicable to the patterns in which the interaction changed dynamically. In that case, the parameters will change corresponding to the change of dynamics that generate the patterns. Therefore, in our model, by monitoring the change of parameters we can detect the anomalous changes of patterns. For example, our model may be useful to detect precursory change of the seismic activity patterns (HIRATA and IMOTO, 1997; POSADAS *et al.*, 2000). Our model is easily extended to the more complicated one. In this study, the states at time step t_n are used on the small template (Fig. 2). The time axis can be extended to t_{n-1} , t_{n-2} , \cdots . We can also extend the range of the cells. In the model, only nearest neighbor cells are considered. To consider second nearest neighbor is another extention. However, we must note that these extention is needed for more observational data set in optimizing the parameters and a lot of parameters to fit (HIRATA *et al.*, 2000b). Our simple model has only three model parameters so that we can easily monitor the change of the patterns. Our model is not special model but a general model for spatio-temporal patterns, which means the model can be applied to various phenomena.

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