Analysis Method depending on Bayes' Theorem for Agent-Based Simulations

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Abstract. This paper proposes the analysis method depending on Bayes' theorem to investigate the probability of cause from simulation results for the agent-based model, aim at calculating an uncertainty and a robustness of simulation results. This investigation has revealed the following implications: (1) the uncertainty and robustness of simulation results derive the divergence and the convergence of point as total structure by the scatter diagram; (2) the uncertainty and robustness of simulation results derive the dissimilarity and the similarity of model's parameters as partial structure by the dendrogram.

1 Introduction

The validation of computational models and simulation results is a critical issue in agent-based simulation because simulation results are very sensitive to how agents are designed and to the model's parameters. There are three "model-to-model" approaches to evaluate the computer model and simulation results. The alignment of computational models and the cross-element validation method validate investigating computational models whether different models can produce the same results after changing an element [1] [2]. The quantitative method compares different simulation results after changing the parameter of agent-based model [3]. Various analysis methods are used a tools depending on the purpose.

The interaction between individual agents can made the phenomena of a system, and has been applied to artificial life and computational economics. The agent-based model resembles ecological system, which also consist of interaction between individuals. The measurement of ecological system are almost invariably subject to error because they are complex [4], this has been called "the uncertainty of ecological system". In the same way, agent-based simulations also produce dynamic and uncertain phenomena. The analysis method needs the Bayes' theorem to calculate the uncertainty from simulation results. This paper proposes an analysis method using Bayes' theorem to investigate the probability of cause using model's parameters from simulation results.

This paper is organized as follows. Section 2 proposes the analysis method using Bayes' theorem, and Section 3 explains the agent-based model using an example of the participant nations in the international trading market. Experiments are reported in Section 4. Section 5 discusses the analysis method using the simulation results. Our conclusions are given in Section 6.

2 Analysis Method using Bayes' Theorem

The data of simulation results and the ecological system compares in the coordinate system and statistical methods to distinguish true responses. On the other hand, the simulation result can compare the phenomenon of past data, and cannot compare future practical data at this point in time. In addition, there are two issues. First, the statistical methods actually represent the probability of obtaining the data given the hypotheses. Second, the comparison of time series data is difficult whether to be similar data of model's parameters in market simulation. In order to overcome these issues, this paper classifies to infer the probability of case by model's parameters from simulation results.

The analysis method consists of the inference using Bayes' theorem and the classification of the probability of cause. The following section explains simplified algorithm of these analysis method to investigate the probability of cause using model's parameters from simulation results.

2.1 Inference using Bayes' Theorem

Overview of Inference using Bayes' Theorem Ecologists regard the truth as uncertain and attempt to use science to gain an improved understanding of the truth, such an approach is consistent with Bayes' theorem by Thomas Bayes [4]. Bayes' theorem uses probabilities to assign degrees of belief to hypotheses or parameter values. It is to know the probability of the cause for the phenomenon. In the same way, the researcher does not know the probability of cause using model's parameter for simulation result, but they can observe only a simulation result for the influence of the model's parameter. This analysis method infers the probability of cause of the model's parameter depending on Bayes' theorem from observed simulation results.

Bayes' theorem combines four components of knowledge. Prior knowledge (prior probability) and new data are combined using an analysis model to produce posterior knowledge (posterior probability). These four components may be represented as:

$$\text{Prior} \times \text{Data} \overset{\text{Analysis Model}}{\longrightarrow} \text{Posterior} \tag{1}$$

The following procedure explains the feature extraction of the simulation result using this concept (Bayes' theorem) in equation (1). Since the simulation result is uncertain in advance, the detailed explanation assumes normal distribution.

1. Choose an analysis model and set prior knowledge (prior probability)
2. The new data collect a simulation result
3. Calculate posterior knowledge (posterior probability) from the prior knowledge (prior probability) and the new data

To understand the above sequence, the detailed is described sequence as follows.

Prior Probability Since the posterior probability calculate from the prior probability and the new data by inference, an uninformative prior for the simulation results use very wide normal distribution (*i.e.*, mean of zero, standard deviation of 1000) and is one in which the data dominates the posterior. The data of observation y from a normal distribution parameterized by a mean θ and a variance σ^2. The prior probability $p(\theta)$ indicates as follows.

$$p(\theta) = \frac{1}{\sqrt{2\pi\tau_0^2}} \exp\left(-\frac{(\theta-\mu_0)^2}{2\tau_0^2}\right) \tag{2}$$

That is, $\theta \sim N(\mu_0, \tau_0^2)$, with hyper-parameters μ_0 and τ_0^2. It means the mean of prior probability μ_0 and the variance of prior probability τ_0^2.

New Data The data of observation y from a normal distribution parameterized by a mean θ and a variance σ^2. The conditional probability $p(y|\theta)$ indicates as follows.

$$p(y|\theta) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\theta)^2}{2\sigma^2}\right) \tag{3}$$

Posterior Probability The posterior probability indicates as following equation (4) using Bayesian analysis and the identically distributed observation $y = (y_1, \ldots, y_n)$. The posterior probability $p(y|\theta)$ indicates as follows.

$$\begin{aligned} p(\theta|y) &\propto p(\theta)p(y|\theta) \\ &= p(\theta)\prod_{i=1}^{n} p(yi|\theta) \\ &\propto \exp\left(-\frac{1}{2}\left[\frac{1}{\tau_0^2}(\theta-\mu_0)^2 + \frac{1}{\sigma^2}\sum_{1}^{n}(y_i-\theta)^2\right]\right) \end{aligned} \tag{4}$$

The data of multiple observation ($y = (y_1 \cdots, y_n)$) from a normal distribution parameterized by the mean μ_n and the variance τ_n^2 of posterior probability [5].

$$p(\theta|y_1 \cdots, y_n) = p(\theta|\overline{y}) = N(\theta|\mu_n, \tau_n^2) \tag{5}$$

$$\mu_n = \frac{\frac{1}{\tau_0^2}\mu_0 + \frac{n}{\sigma^2}\overline{y}}{\frac{1}{\tau_0^2} + \frac{n}{\sigma^2}} \tag{6}$$

$$\frac{1}{\tau_n^2} = \frac{1}{\tau_0^2} + \frac{n}{\sigma^2} \tag{7}$$

The uncertainty and robustness of simulation results indicates the mean and variance by normal probability.

2.2 Classification of Probability of Cause

The classification methods consist of the distance measure and the visualization technique to compare the uncertainty and robustness of simulation results. The distance measure and the visualization technique use as a part of the quantitative method [3].

Distance Measure The distance measure uses the Mahalanobis generalized distance [6] to evaluate the difference between two distributions of simulation results. Each simulation result is mapped to an n-dimensional feature space by employing the feature extraction. It takes into account not only the mean values of the data set but also the correlations of the data set and is scale-invariant. The Mahalanobis generalized distance is defined as:

$$D_M^2(m_1, m_2) = (m_1 - m_2)^t \Sigma_w^{-1} (m_1 - m_2) \tag{8}$$

where m_1 and m_2 are mean vectors of two distributions and Σ_w refers to the within-class covariance matrix that is defined as:

$$\begin{aligned} \Sigma_w &= \sum_{t=1,2} P(wi)\Sigma_i \\ &= \sum_{t=1,2} \left(P(wi)\frac{1}{n_i} \sum_{x \in \chi_i} (x - m_i)(x - m_i)^t \right) \end{aligned} \tag{9}$$

where $P(w_i)$ and x are a priori probability of and feature vector in class w_i, respectively. If the number of samples (simulation results) in classes w_1 and w_2 are identical, then the relation $P(w_1) = P(w_2) = \frac{1}{2}$ holds.

This comparison method can evaluate the difference distributions to measure the distance between every two distributions and construct a distance matrix such as that shown below.

$$M_d = \begin{array}{c} \\ 1 \\ 2 \\ \vdots \\ n \end{array} \begin{array}{c} \begin{array}{cccc} 1 & 2 & \cdots & n \end{array} \\ \begin{pmatrix} 0 & d_{12} & \cdots & d_{1n} \\ d_{21} & 0 & \cdots & d_{2n} \\ \vdots & & \ddots & \vdots \\ d_{n1} & d_{n2} & \cdots & 0 \end{pmatrix} \end{array} \tag{10}$$

Here, d_{ij} represents the distance between distributions i and j; further, $d_{ij} = d_{ji}$ and $d_{ii} = 0$.

Visualization Technique In order to analyze the results of the comparison of models and to examine the validation of models, it is important to visualize the similarities and dissimilarities among multiple distributions. Generally, the distance between two points $P_i(x_i, y_i)$ and $P_j(x_j, y_j)$ is defined as

$$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2} \tag{11}$$

The distance can be computed uniquely when the coordinates of the two points are given. However, the coordinates of two points cannot be determined uniquely when only the distance between the points is known. Multidimensional scaling (MDS) is one of the solution methods for obtaining the coordinates of points from the distance between the points [7]. From the result of MDS, the points can be visualized in a geometric space of low dimensionality (usually, two-dimensional space). Using this visualization technique, the similarities and dissimilarities between different distributions are determined as follows.

$$z_{ij} = -\frac{1}{2}\left(d_{ij}^2 - \sum_{i=1}^{n}\frac{d_{ij}^2}{n} - \sum_{j=1}^{n}\frac{d_{ij}^2}{n} + \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{d_{ij}^2}{n^2}\right) \tag{12}$$

In the above equation, z_{ij} indicates the inner product matrix with coordinates, and d_{ij} indicates the distance between two points of i and j. n indicates the n-dimension in distance matrix.

3 Model

3.1 Agent-based Model of Emission Trading

In the thirteenth session of the conference on the climate change convention, U.S.A announced the reduction of the carbon emission in the post-2012 and the participant nations agree with setting their carbon reduction targets according to Kyoto Protocol [8]. To achieve the targets, the buyer participant nations who do not have enough emission rights have to transact with the seller participant nations who have surplus emission rights in the emissions trading market or they have to reduce the domestic carbon emission by themselves. However, since it is generally difficult for all of the participant nations to succeed in reducing the amount of emission through the emission trading, the current compliance mechanisms have been examined [9]. The agents in our model [10] was designed as the participant nations that agree with Kyoto Protocol to investigate the price fluctuations. Since this simulation results are difficult whether to be similar and dissimilar price fluctuations after changing model's parameters, this paper investigate the probability of cause using model's parameters.

Our model is composed of a lot of adaptive agents that buy and sell their emission rights to achieve their emission reduction targets, which determines the market price as shown in of Fig. 1. Concretely, the agents select their own actions from the possible actions (*i.e.,* the buying, selling, and domestic emission reduction) every month t, and the result derived by the selected actions is evaluated every commitment period defined by five years T as the same as the real international emission trading.

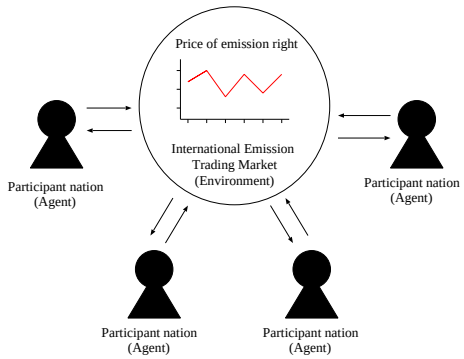

Fig. 1. Participant nation and emissions trading

The agent consists of the two components (*i.e.*, the *rule set* composed of a lot of state-action pairs and the *evaluation function*) and two valuables (*i.e.*, the *emission right* and the *amount of emission*) as shown in Fig. 2. Since the agents aim at achieving their targets through the emission trading or reducing their own domestic emission, we employ the *reinforcement learning* [11] that enables the agents to maximize them reward defined by the successful degree of the emission trading. Concretely, Q-learning [12] is employed as the one of the major reinforcement learning mechanisms. The brief sequence of Fig. 2 is shown as follows.

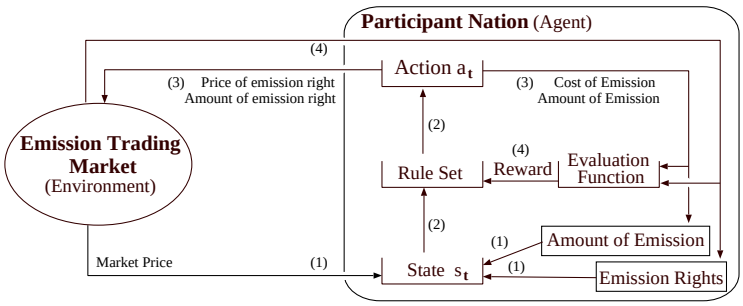

Fig. 2. Decision-making of participant nation (agent)

(1) State acquisition

The agent recognizes the market price, its amount of emission and its emission right.

(2) Action selection by rule set
The agent determines one action from the rule set by selecting either of buying/selling the emission right or reducing the domestic emission to achieve the reduction target determined beforehand.

(3) Buying/selling in the emission trading or reducing the domestic emission
When deciding to buy or sell the emission right, both buying and selling prices of the agents are determined by the auction mechanism. When deciding to reduce the domestic emission, on the other hand, the amount of emission is reduced in the country of the agents.

(4) Changing weight of rule set
When buying or selling the emission right, the agents evaluate their amount of the emission rights changed by the buying and selling transaction, and updates the weight of the selected rule according to the evaluation function. When reducing the domestic emission, on the other hand, the agents evaluate their amount of emission and update the weight of the selected rule according to the evaluation function.

3.2 Compliance Mechanism

The compliance mechanism of Kyoto Protocol is employed in the real emission trading market to promote the participant nations to reduce their greenhouse gas emission. Since Kyoto Protocol establishes legally the binding commitment for reducing the greenhouse gases, the participant nations that agree with Kyoto Protocol have to set their own emission reduction targets to achieve them. To evaluate the achievement of the emission reduction targets of the participant nations, the compliance mechanism checks the participant nation by comparing its total emission right with its total amount of emission at the commitment period of five years.

There are two kinds of the compliance mechanism of Kyoto Protocol [8]. Firstly, the compliance mechanism reduces the amount of the assigned emission right of the participant nations that cannot achieve their targets in the current commitment period. Secondly, it prohibits the participant nations that cannot achieve their targets to sell the emission right to other participant nations in the next commitment period. Since the target can be achieved not only by buying the emission right from other participant nations but also by directly reducing the domestic gas emission, the participant nation has to decide either of actions (*i.e.*, the emission right purchase or the domestic gas emission reduction). Concretely, the total amount of emission and the emission right of every five years are calculated as follows, where T and t indicate the total of five years (corresponding to 60 months) and one month, respectively:

$$TofE_T = \sum_{t=1}^{T} Emission_t \tag{13}$$

$$TofER_T = \sum_{t=1}^{T} Right_t \tag{14}$$

In the above equation, $TofE_T$ and $TofER_T$ indicate the total summation of the month carbon emission $Emission_t$, and the total summation of the month emission right $Right_t$ during the commitment period T (*i.e.*, five years), respectively. When the amount of emission of the participant nations does not exceed the emission right in the current commitment period, the ordinary emission trading (*i.e.*, the buying and selling the emission right) can be carried out in the next commitment period, otherwise the participant nations are restricted in their actions (*i.e.*, they can only reduce their domestic carbon emission or buy the emission right from others) in the next commitment period.

The greenhouse gas emission $Emission_t$ and the emission right $Right_t$ are respectively defined as the following equations (15), (16) and (17).

$$Emission_t = E_t - DR_t \tag{15}$$

$$Right_t = AAU_t \pm ET_t \tag{16}$$

$$AAU_T = Eyear_{1990} \times 5 \times (1 + Target)^{1+T} \tag{17}$$

In these equations, $Emission_t$, E_t, and DR_t indicate the amount of emission of the participant nation in the t-th month, the carbon emission generated in the t-th month, and the amount of the carbon domestic reduction by the participant nation in the t-th month, respectively. $Rights_t$, AAU_t, and ET_t indicate the emission right of the participant nation in the t-th month, the t-th month of the assigned amount unit of the emission right (*i.e.*, $AAU_T \div 60$ month), and the buying and selling results in the t-th month emission trading, respectively. Finally, AAU_T, $Eyear_{1990}$, and $Target$ indicate the assigned amount unit of the emission right of five years, the amount of emission in the base year (1990), and the carbon emission reduction target of the participant nations, respectively.

4 Experiments on Emissions Trading Market

4.1 Cases

To investigate the probability of cause using an model's parameters using Bayes' theorems from simulation results, all agents in the experiments have the model's parameters of the same emission reduction targets of which are investigated under the compliance and non-compliance mechanisms using the parameters as shown in Table 1.

In Table 1, the number of participant nations is set as 39 according to Kyoto Protocol, *i.e.*, the participant nations of the post-2012 including U.S.A. $Eyear_{1990}$ indicates the amount of emission in 1990's data and E_t indicates the amount of emission generated by one nation. Finally, the rate of the penalty reduction $Pdeg$ is set according to Kyoto Protocol. Note that $Eyear_{1990}$ and E_T are tentative value, but such variable setting is enough to investigate the tendency of the emission trading market. The learning rate α, discount rate γ and ϵ for the ϵ-greedy action selection are set as shown in Table 1 which were checked in advance to converge Q-tables of the agents.

The simulation results are averaged from ten runs of simulations. In one run, the simulations are conducted until 10000 iterations (700 months in one iteration) to converge Q-tables of the agents.

Table 1. Parameters of participant nation, compliance mechanism, Q-Learning

Parameter	Value
Number of participant nations	39
Emissions of base year $Eyear_{1990}$	1000
Emissions of one month E_t	65
Rate of penalty reduction $Pdeg$	1.3
Learning rate (step-size parameter) α	0.1
Discount rate γ	0.9
ϵ (for ϵ-greedy action selection)	0.2

4.2 Experiment Results

The purpose of this experiment is to investigate the uncertainty and robustness by employing different model's parameters. This experiment sets compliance mechanism and reduction targets as the difference parameter, and gets market price data of time series in the emissions trading. The parameters set reduction targets $Target$ from 1% to 10% and compliance mechanism or non-compliance mechanism to influence the simulation results. The other parameters were the same in both cases.

Figures 3 and 4 show the classification of multidimensional scaling and cluster analysis using the probability of cause with Bayes' theorem. In figures 3 and 4, "n-" denotes non-compliance mechanism of parameters, "c-" denotes compliance mechanism of parameters and "number" denotes the reduction targets of parameter (For example, "c-10" denotes simulation results of reduction targets 10% of 39s agents with compliance mechanism).

From figure 3, the experiment results obtain the following knowledge through scatter diagram. Since the experiment results are the convergence of point(*i.e.*, c-2, n-2, n-3, $\cdots$,n-10), the simulation results on the agent-based model are the

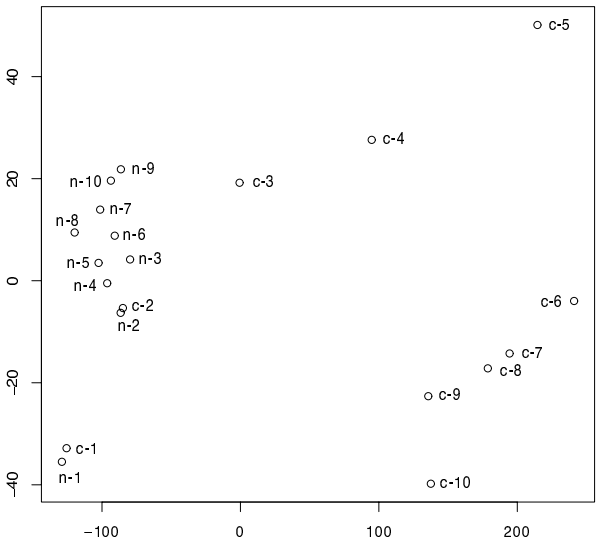

Fig. 3. Scatter diagram using Multidimensional scaling

robustness. Since the experiment results are the divergence of point(*i.e.*, c-2, c-4, c-5), the simulation results on the agent-based model are the uncertainty.

The experiment of figure 3 show similar degree of the simulation result by distance, it is the classification by the visual criterion of the researcher. Since the cluster analysis classify the similar simulation results by the criterion, we classify multiple simulation results from the distance matrix shown in equation 10. On the other hand, this experiment is the lack of guidelines for selecting a threshold value to cut the dendrogram, but we can classify simulation results by the objective criterion.

Figure 4 shows the result of cluster analysis. We cut the dendrogram at a threshold value of Hight = 8 and obtain two clusters. The right cluster shows simulation results with compliance mechanism and high reduction targets of agent. The left cluster shows simulation results compound with compliance mechanism and non-compliance. Since it is difficult to classify the influence of two parameters (the reduction targets, the compliance mechanism), the multiple simulation results is classified by this experiment.

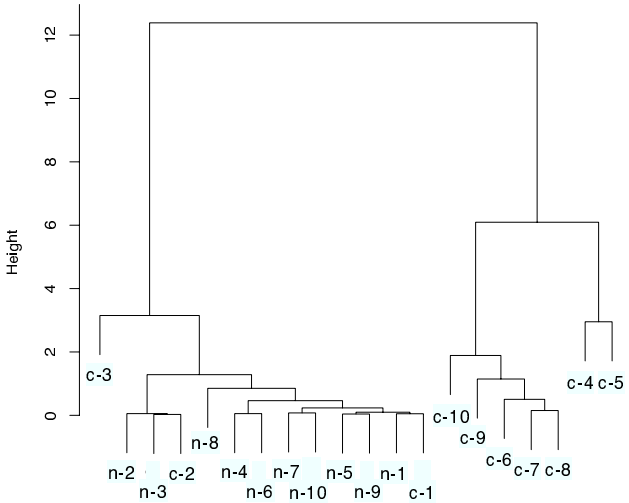

Fig. 4. Dendrogram using cluster analysis

5 Discussion

In Section 4.2, the uncertainty and robustness of simulation results were investigated from multiple viewpoint by the scatter diagram and the dendrogram. The scatter diagram and the dendrogram are technique to represent the essential feature of data. Since the scatter diagram and the dendrogram show total structure and partial structure, the two classification methods need to use together [13]. For example, "c-4" and "c-5" of model's parameters differ the uncertainty and robustness on the two classification methods in Figs. 3 and 4. This analysis method is necessary technique to consider the simulation results in all its aspects.

The proposed analysis method depending on Bayes' theorem calculates the uncertainty and robustness by the probability, and classifies by the classification methods. The statistics (frequency probability methods) and this analysis method use the probability distribution. Two method differ the notion of probability. Statistical methods (frequency probability methods) make the interpretation of data repeatable [4]. This analysis method is calculation of the probability of a hypothesis being true in uncertainty of the parameter value. In other words, the probability distribution represents the uncertainty and the robustness from simulation results in uncertain phenomena.

6 Conclusion

This paper focused on the analyses method using Bayes' theorem to calculate the uncertainty and robustness of simulation results. For this purpose, this research investigate the probability of cause from simulation results, and compared the uncertainty and robustness by the scatter diagram and the dendrogram. This investigation has revealed the following implications: (1) the uncertainty and robustness of simulation results show the divergence and the convergence of point as total structure by the scatter diagram; (2) the uncertainty and robustness of simulation results show the dissimilarity and the similarity of model's parameters as partial structure by the dendrogram. This analysis method derives the uncertainty and the robustness of simulation results with the multiple viewpoints.

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