2004－ICS－138 (31)
2004／12／6

Scientific Discovery of Dynamic Hidden States and Differential Law Equations

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This paper proposes a novel appropach to discover dynamic hidden states and simultaneous time differential law equations from time series data observed in an objective process. This task has not been addressed in the past work though it is essentially important in scientific discovery since any behaviors of objective processes emerge in time evolution. The promising performance of the proposed approach is demonstrated through the analysis of synthetic data.

1. Introduction

Many of the conventional approaches to identify numerical models from measurement data, *e.g.*, system identification theory[1] and artificial neural network[2], derive an "*asymptotic model*" of an objective process over a narrow range of its state. Their plausibility is based on the assumption that the characteristics of the objective process over the state range can be sufficiently well captured by the presumed structure of the adopted equations such as linear and/or logistic formulae. However, this assumption usually does not hold over a wide range of states in the objective process because the presumed structure is merely an approximation within the narrow range. Accordingly the conventional approaches usually do not identify the law equations to represent the first principles governing the objective process over a wide state range.

In contrast, the main goal of scientific law equation discovery is to discover the first principle based law equations from measurement data. The most well known pioneering system to discover scientific law equations is BACON[3]. This system searches for a "*complete equation*" governing the data measured in a continuous process, where the complete equation is an equation constraining n quantities with $n-1$ degree of freedom ☆. It tries to figure out an invariant and its associated relation between two quantities over a wide state range by bi-variate fitting under a given laboratory experiment where some quantities are actively controlled. The found bi-variate relations are successively composed with the other relations, and finally a complete equation representing the multiple measurement quantities is resulted. FAHRENHEIT[4], ABACUS[5] and IDS[6] are the successors that use basically similar algorithms to BACON in searching for a complete equation.

However, one of the drawbacks of the BACON family is the low likeliness to discover the equations representing the first principles underlying the objective process, since they do not use any criteria to capture constraints induced by the first principles. The second drawback is so high time complexity due to the unconstrained search space of equation formulae that equations contain only a few quantities can be searched within a tractable time. The third drawback is the considerable amount of ambiguity in their results for noisy data even for the equations containing a few quantities[7),8]. To alleviate these difficulties, some systems, e.g. FAHRENHEIT, ABACUS and COPER[9], introduced some naive constraints imposed by unit dimension of quantities to prune the meaningless solutions. An example of the constraints is the "*dimensional homogeneity*" that every terms in a candidate law equation must have an identical unit, otherwise it is pruned. A problem of this approach is its narrow applicability only to the quantities whose units are clearly known. To further overcome this difficulty, SDS has proposed [10]. It discovers scientific law equations by limiting its search space to mathematically admissible equations in terms of the constraints of "*scale-type*" and "*identity*". These constraints come from the basic charac-

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☆ The equation ${x_1}^2 + {x_2}^2 + ... + {x_n}^2 = 0$ is not complete, since the values of all n quantities is 0, i.e., n quantities are constrained with no degree of freedom. On the other hand, $x_1 + x_2 + ... + x_n = 0$ is complete.

teristics of the quantities' definitions and the relations necessarily standing in the objective processes. The admissible equations discovered by SDS are considered to represent plausible relations among quantities reflecting the first principles governing the objective process. The detailed characterization of the first principle equations can be seen elsewhere[11]. Since the knowledge of scale-types is widely obtained in various domains, SDS is applicable to non-physical domains including biology, sociology, and economics. In addition, an extra strong mathematical constraint named triplet checking is introduced to check the validity of those bi-variate equations. By these constraints, the complexity of the algorithm remains quite low, and the high robustness against the noise in the measurements is provided.

The power of the systems must be further extended to discover scientific law equations in real world. An issue is to discover "*multiple equations*" governing given measurement data. This is because the most of the real world processes consist of multiple mechanisms, and are represented by multiple equations in terms of given quantities. Some past studies have partially addressed this issue. The aforementioned FAHRENHEIT and ABACUS identify each operation mode of the objective process and transition conditions among these modes, and they derives an equation to represent each mode. For example, they can discover state equations of water for solid, liquid and gas phases respectively from experimental data. However, many processes such as large scale electric circuits are represented by "*simultaneous equations*". The model representation in form of simultaneous equations is essential to grasp the dependency structure among the multiple mechanisms in the processes[12),13]. To address this issue, SSF has been proposed to discover a valid simultaneous equation structure governing the objective process based on the identification of "*minimal complete subsets*" of simultaneous equations embedded in data measured under experimental environments[14]. SSF combined with SDS enables the discovery of quantitative simultaneous law equation models.

The second issue is the ability to discover law equations under "passive observations." The aforementioned approaches require interactions to control and measure the objective process states under experimental environments. However, the number of controllable quantities is quite limited, and even none of them are controllable due to some practical reasons in many scientific and engineering domains. For instance, the astronomical experiments to control the parameters of fusion reactions in distant huge stars are impossible. The economical experiments to cause financial panics are unacceptable for our society. The discovery of the first principle equations under the passive observation will play highly important role to understand the fundamental mechanisms underlying the variety of the objective processes. Only a limited number of law equation discovery systems have addressed the application to passively observed data. The aforementioned SDS and SSF have been extended to be applicable to the passively observed data by introducing novel principles of "*quasi-bi-variate fitting*"[15] and "*quasi-experiment on dependency*"[16] which identify the dependency and the bi-variate relations among quantities under the passively observed data without performing actual experiment. It demonstrated excellent features of the robustness against observation noise and the limited computational complexity.

The third issue is to discover "*simultaneous time differential equations*" reflecting the first principles governing the dynamics of objective processes. This task plays a highly important role in scientific discovery, since any behaviors of objective processes emerge in time evolution under their first principles. However, all aforementioned approaches are limited to discover law equations representing static behaviors of objective processes. An effort to develop a law equation discovery system called LAGRANGE has been made to automatically discover dynamic models represented by simultaneous time differential equations[17]. It can discover the model equations from passively observed time series data based on an ILP-like generate and test reasoning on an objective process. Its drawback is very high complexity of the search since vast number of the candidate equation formulae are generated and tested. Subsequently, its further extended version called LAGRAMGE was developed to introduce background knowledge in the domain of the objective process[18]. The introduction of the appropriate domain knowledge can efficiently limit the search space of the equations and provide the right model equations of the first principles underlying the objective processes. However, the right model equations may be missed in the search, if the given background knowledge is inappropriate.

Its more essential limit is the lack of the ability to discover "*hidden state quantities*," because it assumes the direct observation of all quantities representing states required to model the dynamics of the objective process. For example, consider a rocket having its mass M [kg] and producing its thrust by the fuel jet of m [kg/sec] and v [m/sec] in space. Then its dynamics is represented by the following three time differential equations.

$$\frac{dV}{dt} = \frac{mv}{M}, \frac{dX}{dt} = V, \text{ and } \frac{dM}{dt} = -m,$$

where V [m/sec] and X [m] are the velocity and the position of the rocket. m and v are the parameters known from the design specification of the rocket. X and V can be measured from the outside of the rocket. But M is not observable unless the rocket has a specific mass sensor. In fact, the measurement of M for a real space rocket is so hard that it must be indirectly estimated from the measurement of X and V. In this case, M is called a hidden state quantity since it is unobservable but has its independent dynamics represented by the third differential equation. Without any background domain knowledge, we do not know the number of hidden state quantities, *i.e.*, the number of differential equations to be required to model the objective process. The identification of the hidden state quantities from observed data is an essential task to discover the simultaneous time differential equations reflecting the first principles underlying the objective process.

In this paper, we propose a novel method to discover a model of an objective process having the following features.

(1) The model is a simultaneous time differential equations representing the dynamic behavior of an objective process.
(2) The model is not an asymptotic approximated model but an model representing the first principles governing the objective process.
(3) The model can include hidden state quantities and their governing differential equations.
(4) The model is discovered without using background domain knowledge specific to the objective process.
(5) The model is discovered from passively observed data.

First, our proposing scientific equation discovery approach is outlined. Second the performance evaluation of our approach through numerical experiments on synthetic data is shown.

2. Discovery Method

2.1 Basic Problem Setting

We adopt the following "*state space expression*" to model objective processes and measurements without loss of generality.

$$\dot{\boldsymbol{x}} = \boldsymbol{h}(\boldsymbol{x}) + \boldsymbol{v} \quad (\boldsymbol{v} \sim N(0, \Sigma_v)), \text{ and}$$
$$\boldsymbol{y}(\boldsymbol{k}) = \boldsymbol{C}\boldsymbol{x}(\boldsymbol{k}) + \boldsymbol{w}(\boldsymbol{k}) \quad (\boldsymbol{w}(\boldsymbol{k}) \sim N(0, \Sigma_w)),$$

where the first equation is called a "*transition equation*" and the second a "*measurement equation*." $\boldsymbol{x}$ is called a "*state vector*", $\boldsymbol{h}$ a transition function, $\boldsymbol{v}$ a process noise vector, $\boldsymbol{y}$ a measurement vector, $\boldsymbol{C}$ a measurement matrix, and $\boldsymbol{w}$ a measurement noise k a time index. $\boldsymbol{h}$ is nonlinear in general, and any state transition of $\boldsymbol{x}$ can be represented by this formulation. While $\boldsymbol{C}$ is a linear transformation representing measurement facilities to derive the measurement quantities in $\boldsymbol{y}$ from the state quantities in $\boldsymbol{x}$, the facilities are artificial and linear in most cases. Thus, this does not reduce the generality of this expression. If $\boldsymbol{C}$ is a unit matrix, all state quantities are directly observable through the measurement. However, if $\boldsymbol{C}$ is not full rank, some state quantities may not be directly observed. Such state quantities are called "*hidden state quantities.*" The aforementioned mass of the rocket M is an example of this hidden state quantity. $\boldsymbol{C}$ is generally known since it is artificial, whereas $\boldsymbol{h}$ and some elements of $\boldsymbol{x}$ are unknown. Our proposing method identifies the number of elements in $\boldsymbol{x}$, *i.e.*, the dimension of $\boldsymbol{x}$ from given measurement data at first. Subsequently, it searches $\boldsymbol{h}$ based on the data within mathematically admissible formulae.

2.2 Outline of Approach

The approach is outlined in Fig. 1. Given a set of measurement data and knowledge on

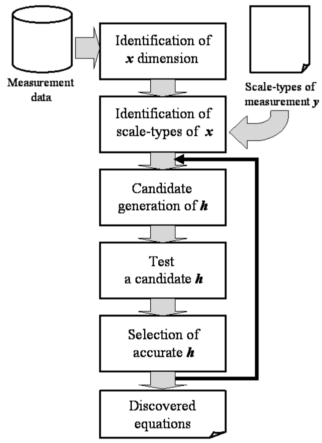

Fig. 1 Block Diagram of Approach.

scale-types of measurement quantities, the dimension of $\boldsymbol{x}$ is identified through a statistical analysis called "*correlation dimension analysis*." The measured values of $\boldsymbol{y(k)}$ are mapped to a phase space of time delayed trajectory, and the degree of freedom embedded in measured time evolution behavior is estimated by computing the relation between a time lag and the time lagged correlation. Once the dimension of $\boldsymbol{x}$ is known, scale-types of the elements in $\boldsymbol{x}$ are estimated as many as possible based on scale-type constraints and the information of the scale-types of the elements in $\boldsymbol{y}$. The scale-type constraints are mathematical admissibility condition on the relation among measured quantities by the nature of the measurement process. Once the scale-types of the elements in $\boldsymbol{x}$ are obtained, the candidate equation formulae of $\boldsymbol{h}$ admissible by the scale-type constraints are generated, and the validity of the candidate is tested through a certain tracking simulation on the given measurement data which is called a "*particle filter*" approach. Then, the candidate $\boldsymbol{h}$ providing highly accurate tracking, in terms of "*mean square error* (MSE)" is selected through the iteration of the candidate generation and testing. Finally, the most accurate $\boldsymbol{h}$ in the data tacking simulation is selected as the discovered dynamic model of the objective process.

3. Performance Evaluation

The performance of our proposing approach has been evaluated through two types of numerical experiments using synthetic data. One is to evaluate the basic search of candidate equations through the generation and test approach. A dynamic behavior of an objective system is simulated, and the time series data of measurement quantities which are the direct observation of all state quantities of the objective system are recorded. Hence, no hidden state exits. Another is to evaluate the ability to discover a hidden state quantity in correlation dimension analysis and the search of candidate equations including the hidden state quantity. Time series data recorded in the simulation are the measurement quantities on a part of the state quantities. In each simulation, measurement noise $\boldsymbol{w}$ having 0.1% relative amplitude of the measurement $\boldsymbol{y}$ is introduced to evaluate the robustness of the approach against noise distortion whereas the process noise $\boldsymbol{v}$ is set to be negligible. A personal computer having 2.0GHz Pentium IV and 1GB main memory was used for the simulation and the evaluation.

3.1 Evaluation of Basic Search

First ,the approach is applied to the time series data of the measurement quantities produced by the simulation of the following two dimensional nonlinear system, where the scale-types of both y_1 and y_2 are ratio scale, and those of x_1 and x_2 are also ratio scale.

Transition Equation

$$\frac{dx_1}{dt} = -0.5x_1 \qquad (x_1(0) = -1),$$
$$\frac{dx_2}{dt} = x_1x_2 \qquad (x_2(0) = 1), \text{ and}$$

Measurement Equation

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}. \qquad (1)$$

Table 1 shows the top five results of the discovered transition equation in the ascending order of MSE. The top four show the successful discovery of the original equations. The values of MSE are almost comparable with the amplitude of the measurement noise which is 1.0×10^{-6}. The required computation time to complete the search was almost three days.

Next, the approach is applied to the time series data of the measurement quantities produced by the simulation of the following two dimensional nonlinear system, where the scale-types of y_1 and x_1 are ratio scale, and those of y_2 and x_2 are interval scale.

Transition Equation

Table 1 Ratio Scale Observations.

Equations	MSE
$dx_1/dt{=}-0.493x_1$ $dx_2/dt{=}1.04x_1x_2$	2.626×10^{-6}
$dx_1/dt{=}-0.512x_1$ $dx_2/dt{=}0.932x_1x_2$	2.729×10^{-6}
$dx_1/dt{=}-0.523x_1$ $dx_2/dt{=}1.03x_1x_2$	2.717×10^{-6}
$dx_1/dt{=}-0.530x_1$ $dx_2/dt{=}0.972x_1x_2$	2.757×10^{-6}
$dx_1/dt{=}-0.512x_1$ $dx_2/dt{=}-0.819x_2^2$	1.477×10^{-5}

Results are in the ascending order of MSE.

Table 2 Ratio and Interval Scale Observations.

Equations	MSE
$dx_1/dt{=}0.026x_1(x_2{+}5.470)$ $dx_2/dt{=}-0.073(x_2{+}0.532)$	5.320×10^{-5}
$dx_1/dt{=}0.059(x_2{+}1.428)^{-3}$ $dx_2/dt{=}-0.055$	1.125×10^{-4}
$dx_1/dt{=}0.376x_1(x_2{+}0.207)$ $dx_2/dt{=}-0.073x_1 exp(0.680x_2)$	1.231×10^{-4}
$dx_1/dt{=}0.007(x_2{+}1.310)^{-3}$ $dx_2/dt{=}0.004x_1$	4.945×10^{-4}
$dx_1/dt{=}-0.365x_1(x_2{+}5.962)^{-2}$ $dx_2/dt{=}-0.004x_1$	5.690×10^{-4}

Results are in the ascending order of MSE.

$$\frac{dx_1}{dt} = 0.4x_1(x_2+0.2) \qquad (x_1(0) = -1),$$
$$\frac{dx_2}{dt} = -0.1(x_2+0.6) \qquad (x_2(0) = 1), \text{ and}$$

Measurement Equation

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}. \qquad (2)$$

Table 2 shows the top five results of the discovered transition equation. The top shows the successful discovery of the original equations. The values of MSE are higher than the level of the measurement noise. This may be because the equation search becomes more sensitive to the noise due to the increase of the number of fitting coefficients in the equation. The required computation time to complete the search was almost seventeen days. This is also consistent with the fact that the variety of candidate equation formulae is higher in case of the mixture of ratio and interval scale quantities.

3.2 Evaluation of Hidden State Search

The approach is applied to the time series data of the measurement quantity y_1 produced by the following two dimensional nonlinear system, where the scale-types of y_1 and x_1 are ratio scale, and x_2 is a hidden state quantity.

Transition Equation

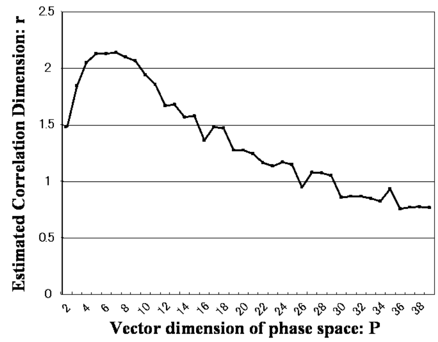

Fig. 2 Correlation Dimension Analysis.

$$\frac{dx_1}{dt} = 0.1x_1x_2 \qquad (x_1(0) = 0.25),$$
$$\frac{dx_2}{dt} = -0.25x_1 \qquad (x_2(0) = 4), \text{ and}$$

Measurement Equation

$$y_1 = \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}. \qquad (3)$$

Because the number of the hidden state quantities and their time differential equations is not known in advance without the knowledge of the simulation, the correlation dimension analysis is applied first. Figure 2 is the plot of vector dimension of phase space P vs. estimated correlation dimension. Because the maximum value of the estimated dimension is 2.14, the dimension of the objective process, *i.e.*, the number of time differential equations is judged to be the nearest integer 2. Consequently, the candidates consisting of two differential equations are search under the scale-type constraint. Table 3 shows the top five results of the search. The top, third and fourth shows the successful discovery of the original transition equation while the coefficients are not very accurate. In contrast, the value of MSE is almost comparable or less than the amplitude of the measurement noise. This is because the less number of measurement quantities allows slight overfitting of the equations, but leads the result more erroneous. The required computation time to complete the search was almost seventeen days. This is consistent with the fact that unknown scale type of the hidden state quantity x_2 significantly increases the variety of candidate equation formulae.

4. Conclusion

We showed a novel method to discover a si-

Table 3 Hidden States and Ratio Scale Observation.

Equations	MSE
$dx_1/dt=0.044x_1x_2$, $dx_2/dt=-0.570x_1$	9.240×10^{-7}
$dx_1/dt=0.15x_1x_2$, $dx_2/dt=-0.245$	9.390×10^{-7}
$dx_1/dt=0.026x_1x_2$, $dx_2/dt=-0.588x_1$	9.550×10^{-7}
$dx_1/dt=0.033x_1x_2$, $dx_2/dt=-0.683x_1$	9.590×10^{-7}
$dx_1/dt=0.098x_1x_2$, $dx_2/dt=-0.033x_1^3x_2^{-1}$	9.660×10^{-7}

Results are in the ascending order of MSE.

multaneous time differential equations representing the first principles governing dynamic behavior of an objective process from passively observed data. The significant features of this approach are the discovery without strong bias of the domain knowledge due to no use of knowledge specific to the objective process and the wide applicability to the cases including hidden state quantities in the objective process. The remained major issue is to overcome the computational time complexity of the search. Under the current environment, the derivation of models consisting of more than a few differential equations are not very practical. The study to significantly increase the search speed is currently underway.

Acknowledgments This research has conducted under the support of JSPS Kiban Kenkyuu (B) (2) 16300045.

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