Development of SDS2: Smart Discovery System for Simultaneous Equation Systems

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Abstract

SDS2 is a system to discover and identify the quantitative model consisting of simultaneous equations reflecting the first principles underlying the objective process through experiments. It consists of SSF and SDS, where the former is to discover the structure of the simultaneous equations and the latter to discover a quantitative formula of each complete equation. The power of SDS2 comes from the use of the complete subset structure in a set of simultaneous equations, the scale-types of the measurement data and the mathematical property of identity by which to constrain the admissible solutions. The basic principles, algorithms and implementation of SDS2 are described, and its efficiency and practicality are demonstrated and discussed with large scale working examples. This work is to promote the research of scientific discovery to a novel and promising direction, since the conventional equation discovery systems could not handle such a simultaneous equation process in a highly efficient manner.

1 Introduction

Number of methods have been proposed to discover quantitative formulae of scientific laws from experimental measurements. Langley and others' BACON systems [1] are the most well known as a pioneering work. FAHRENHEIT [2] and ABACUS [3] are such successors that use basically similar algorithms to BACON in searching for a complete equation governing the measured data. Major drawbacks of the BACON family are their complexity in the search of equation formulae and the considerable amount of ambiguity in their results for noisy data [4] [5]. To alleviate these difficulties, some later systems, e.g. ABACUS and COPER [6], utilize the information of the unit dimension of quantities to prune the meaningless terms. However, their applicability is limited only to the case where the quantity dimension is known.

Another difficulty of the conventional systems to discover a model of practical and large scale process is that such process is represented by multiple equations. Some of the aforementioned systems such as FAHRENHEIT and ABACUS can identify each operation mode of the objective process and derive an equation to represent each mode. For example, they can discover state equations of water for solid, liquid and gas phases respectively. 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 [7] [8]. An effort to develop a system called LAGRANGE has been made to automatically discover dynamical models represented by simultaneous equations[9]. However, it derives many redundant models in high computational complexity while the soundness of the solutions is not guaranteed.

The objective of this study is to develop a new scientific discovery system named "*SDS2 (Smart Discovery System 2)*" which is an extended version of our previous system "*SDS*" [10]. It overcomes the drawbacks of the conventional scientific discovery systems. The main extenstion of SDS2 is to discover a complex model of an objective process represented by a set of simultaneous equations from measured quantities in experiments. SDS2 also inherits the full advantages of SDS such as the wide applicability, the low complexity and the high robustness against the noise.

SDS2 has been developed based on some mathematical principles established in our past research [10] [11] [12]. It consists of "*SSF (Simultaneous System Finder)*" and the main body of SDS, where the former is to discover the structure of the simultaneous equations and the latter to discover a quantitative formula of each complete equation. SDS2 applies SSF to the objectiove process to identify its simultaneous structure at first, and then applies the algorithm of SDS to derive a quantitative formula for each of the identified simultaneous equations. In the following sections, first the outline of the principle and the algorithm of SSF are explained. Second those of SDS are mentioned. Third the implementation of SSF and SDS combined into SDS2 is described, and finally the evaluation of the performance of SDS2 is given.

2 Outline of Principle and Algorithm of SSF

We set two assumptions on the objective process to be analyzed. One is that the objective process can be represented by a set of quantitative, continuous, complete and under-constrained simultaneous equations for the quantity ranges of our interest. Another is that all of the quantities in every equation can be measured, and all of the quantities except one dependent quantity can be controlled in every equation to their arbitrary values in the range under experiments while satisfying the constraints of the other equations. These assumptions are common in the past BACON family except the features associated with the simultaneous equations.

The principles of SSF are explained through a simple electric circuit consisting of two parallel resistances and a battery depicted in Fig. 1. One way of modeling this is by

$$V_1 = I_1 R_1 \text{ [1]}, V_2 = I_2 R_2 \text{ [2]}, V_e = V_1 \text{ [3] and } V_e = V_2 \text{ [4]}, \quad (1)$$

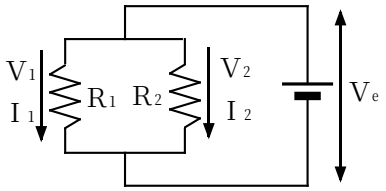

Figure 1: An circuit of parallel resistances.

where R_1, R_2:two resistances, V_1, V_2:voltage differences across the resistances, I_1, I_2:electric current going through the resistances and V_e:voltage of the battery.

The same circuit can be modeled by another set of equations.

$$I_1R_1 = I_2R_2 \text{ [1]}, V_2 = I_2R_2 \text{ [2]}, V_e = V_1 \text{ [3] and } V_e = V_2 \text{ [4]}. \quad (2)$$

Both representations give correct behaviors of the circuit. The configuration of the quantities in a set of simultaneous equations is represented by an "*incidence matrix*" T where its rows $E = \{eq_i | i = 1, ...M\}$ correspond to the mutually independent equations and its columns $Q = \{q_j | j = 1, ..., N\}$ to the quantities. If the j-th quantity appears in the i-th equation, then the (i, j) element of T, i.e., $T_{ij} = 1$, and otherwise $T_{ij} = 0$ [8]. When a subset consisting of n independent equations containing n undetermined quantities are obtained by exogenously specifying the values of some extra quantities in the under-constrained simultaneous equations, the values of those n quantities are determined by solving the equations in the subset. In terms of an incidence matrix, exogenous specification of a quantity value corresponds to eliminating the column of the quantity. Under this consideration, the following definition is introduced.

Definition 1 (complete subset) *Given an incidence matrix T, after applying elimination of a set of columns, $RQ(\subset Q)$, let a set of nonzero columns of $T[CE, Q-RQ]$ be $NQ(\subseteq Q-RQ)$, where $CE \subseteq E$, and $T[CE, Q - RQ]$ is a sub-incidence matrix for equations in CE and quantities in $Q - RQ$. CE is called a "complete subset" of order n, if $|CE| = |NQ| = n$. Here, $|\bullet|$ stands for the cardinality of a set.*

If we exogenously specify the values of V_e and R_1, the first, the third and the forth rows of the matrix for Eq.(1) come to contain the three nonzero columns of V_1, V_2 and I_1. Thus these equations form a complete subset of order 3, and the three quantities are determined while the others, I_2 and R_2, are not. On the other hand, if the identical specification on V_e and R_1 is made in the latter model, no complete subset of order 3 is obtained, since every combination of three rows in the matrix for Eq.(2) contains more than three nonzero columns. In the real electric circuit, the validity of the consequence derived by the former model is clear. The model having the incidence matrix which always derives a valid interpretation in determining the quantities of an objective process is named "*structural form*" in this paper.

When two models mutually have identical complete subsets, the interpretation in those models is also identical, since each complete subset in their matrices represents a mechanism to determine the values of the quantities. The relation between the two models having an identical complete subset is characterized by the following theorem.

Theorem 1 (invariance theorem) *Given a transform $f : U_E \rightarrow U_E$ where U_E is the entire universe of equations. When CE is a complete subset of order n in T, $f(CE)$ is also a complete subset of order n, if $f(CE)$ for $CE \subset U_E$ maintains the number of equations and the nonzero column structure, i.e., $|CE| = |f(CE)|$ and $CQ = CQ_f$, where CQ_f is a set of nonzero columns in $T[f(CE), Q]$.*

Various simultaneous equation formulae maintaining the equivalence of the quantitative relations and the dependency structure can be derived by limiting the transformation f to a

quantitative one satisfying the "*invariance theorem*" such as substitution and arithmetic operation among equations. As the complexity of the algorithm to enumerate all forms of a complete subset admitted by the transform f faces the combinatorial explosion, our approach identifies only one specific form defined bellow.

Definition 2 (canonical form of a complete subset) *Given a complete subset CE of order n, the "canonical form" of CE is the form where all elements of the nonzero columns CQ in its incidence matrix $T[CE, Q]$ are* 1.

Because every admissible form is equivalent to every other, the identification of the canonical form is sufficient, and every other can be derived by applying each appropriate f to the form.

Though each complete subset represents a basic mechanism to determine the values of quantities in given simultaneous equations, some complete subsets are not mutually independent. For instance, the following four complete subsets can be found in the example of Eqs.(1).

$$\{[3],[4]\}(n=2), \quad \{[1],[3],[4]\}(n=3), \quad \{[2],[3],[4]\}(n=3), \quad \{[1],[2],[3],[4]\}(n=4) \tag{3}$$

The number in [ ] indicates each equation and n the order of the subset. They mutually have many overlaps, and the complete subsets having higher orders represent the redundant mechanism with the lower subsets. Thus, the following definitions are introduced to decompose the internal structure of a complete subset.

Definition 3 (independent component of a complete subset) *The independent component DE_i of the complete subset CE_i is defined as*

$$DE_i = CE_i - \bigcup_{\substack{\forall CE_j \subset CE_i \\ \text{and } CE_j \in L}} CE_j.$$

The set of essential quantities DQ_i of CE_i which do not belong to any other smaller complete subsets but are involved only in CE_i is also defined as

$$DQ_i = CQ_i - \bigcup_{\substack{\forall CE_j \subset CE_i \\ \text{and } CE_j \in L}} CQ_j,$$

where CQ_i is a set of nonzero columns of $T(CE_i, Q)$. The order δn_i and the degree of freedom δm_i of DE_i are defined as

$$\delta n_i = |DE_i| \text{ and } \delta m_i = |DQ_i| - |DE_i|.$$

In the example of Eq.(3), the three independent components are derived.

$$\begin{aligned} DE_1 &= \{[3],[4]\} - \phi = \{[3],[4]\}, \quad \delta n_1 = 2 - 0 = 2, \\ DE_2 &= \{[1],[3],[4]\} - \{[3],[4]\} = \{[1]\}, \quad \delta n_2 = 3 - 2 = 1, \\ DE_3 &= \{[2],[3],[4]\} - \{[3],[4]\} = \{[2]\}, \quad \delta n_3 = 3 - 2 = 1. \end{aligned} \tag{4}$$

Because each independent component DE_i is a subset of the complete subset CE_i, the nonzero column structure of DE_i also follows the invariance theorem. Consequently, the subset of the canonical from of CE_i is applicable to represent DE_i. Based on this consideration, the definition of the canonical form of the simultaneous equations is introduced.

Definition 4 (canonical form of simultaneous equations) *The "canonical form" of a set of simultaneous equations consists of the equations in $\cup_{i=1}^{b} DE_i$ where each equation in DE_i is represented by the canonical form in the complete subset CE_i, where b is the total number of DE_i.*

(S1) *Let* $Q = \{q_k | k = 1, ..., N\}$ *be a set of quantities that appear in the model of an objective process. Set* $X = \{x_k | x_k = q_k$, *for all but directly controllable* $q_k \in Q\}$, $DE = \phi$, $DQ = \phi$, $N = \phi$, $M = \phi$, $h = 1$ *and* $i = 1$.

(S2) *Choose* $C_j \subset DQ_j \in DQ$ *for some* DQ_j *and also* $C_x \subseteq X$, *and take their union* $C_{hi} = ... \cup C_j \cup ... \cup C_x$ *while maintaining* $|C_j| \leq \delta m_j$ *and* $|C_{hi}| = h$. *Control all* $x_k \in C_{hi}, k = 1, ..., |C_{hi}|$ *in the experiment.*

(S3) *Let a set of all quantities whose values are determined be* $D_{hi} \subseteq (Q - C_{hi})$ *where* $D_{hi} \neq \phi$. *Set* $DE_{hi} = C_{hi} + D_{hi}$, $DQ_{hi} = DE_{hi} - \cup_{\substack{\forall DE_{h'i'} \subset DE_{hi} \\ DE_{h'i'} \in DE}} DE_{h'i'}$, $\delta n_{hi} = |D_{hi}| - \sum_{\substack{\forall DE_{h'i'} \subset DE_{hi} \\ DE_{h'i'} \in DE}} \delta n_{h'i'}$, *and* $\delta m_{hi} = |DQ_{hi}| - \delta n_{hi}$. *If* $\delta n_{hi} > 0$, *then add* DE_{hi} *to the list* DE, DQ_{hi} *to the list* DQ, δn_{hi} *to the list* N, δm_{hi} *to the list* M *and* $X = X - DQ_{hi}$.

(S4) *If all quantities are determined, i.e.,* $D_{hi} = Q - C_{hi}$, *then go to (S5), else if no more* C_{hi} *where* $|C_{hi}| = h$ *exists, set* $h = h + 1, i = 1$ *and go to (S2), else set* $i = i + 1$ *and go to (S2).*

(S5) *The contents of the lists* DE, DQ *and* N *represent the sets of quantities involved in independent components, the sets of essential quantities and their orders respectively.*

Figure 2: Algorithm for finding structural canonical form

If the canonical form of simultaneous equations are experimentally derived to reflect the actual dependency structure among quantities in the objective process, then the model must be a "*structural form*". Thus, the following terminology is introduced.

Definition 5 (structural canonical form) *If the canonical form of simultaneous equations is derived to be a "structural form", then the form is named "structural canonical form".*

Under our aforementioned assumption on the measurements and the controllability of quantities, a bottom up algorithm described in Fig. 2 has been developed and implemented into SSF. SSF requires a list of the quantities for the modeling of the objective process and their actual measurements. Starting from the set of control quantities having small cardinality, this algorithm tests if values of any quantities become to be fully under control. If such controlled quantities are found, the collection of the control quantities and the controlled quantities are considered as a newly found complete subset $|CE_i|$. Then, based on the definition3, its $|DE_i|$, $|DQ_i|$, δn_i and δm_i are derived and stored. Once any new independent component is derived, only δm_i of the quantities in every $|DQ_i|$ and the quantities which do not belong to any $|DQ_i|$ so far found are used for control. The constraint of $|DQ_i|$ does not miss any complete subset to search due to the monotonic lattice structure among complete subsets.

3 Outline of Principles and Algorithm of SDS

SDS uses the information of scale-types of quantities to discover the formula of each equation. The quantitative scale-types are interval, ratio and absolute scales[13]. Examples of the interval scale quantities are temperature in Celsius and sound tone where the origins of their scales are not absolute, and are changeable by human's definitions. Examples of the ratio scale quantities are physical mass and absolute temperature where each has an absolute origin. The absolute scale quantities are dimensionless quantities.

The properties of the quantities in terms of the scale-types yields "*scale-type constraint*" characterized by the following theorems [10].

Theorem 2 (Extended Buckingham Π-theorem) *If $\phi(x_1, x_2, x_3, ..., x_n) = 0$ is a complete equation, and if each argument is one of interval, ratio and absolute scale-types, then the solution can be written in the form*

$$F(\Pi_1, \Pi_2, ..., \Pi_{n-w}) = 0,$$

where n is the number of arguments of ϕ, w is the basic number of bases in $x_1, x_2, x_3, .., x_n$, respectively. For all i, Π_i is an absolute scale-type quantity.

Bases are such basic factors independent of the other bases in the given ϕ, for instance, as length $[L]$, mass $[M]$, time $[T]$ of physical unit and the origin of temperature in Celsius.

Theorem 3 (Extended Product Theorem) *Assuming primary quantities in a set R are ratio scale-type, and those in another set I are interval scale-type, the function ρ relating $x_i \in R \cup I$ to a secondary quantity Π is constrained to one of the following two:*

$$\Pi = (\prod_{x_i \in R} |x_i|^{a_i})(\prod_{I_k \subseteq I} (\sum_{x_j \in I_k} b_{kj}|x_j| + c_k)^{a_k})$$

$$\Pi = \sum_{x_i \in R} a_i \log|x_i| + \sum_{I_k \subseteq I} a_k \log(\sum_{x_j \in I_k} b_{kj}|x_j| + c_k) + \sum_{x_\ell \in I_g \subseteq I} b_{g\ell}|x_\ell| + c_g$$

where all coefficients except Π are constants and $I_k \cap I_g = \phi$.

These theorems state that any meaningful complete equation consisting only of the arguments of interval, ratio and absolute scale-types can be decomposed into an equation of absolute scale-type quantities having an arbitrary form and equations of interval and ratio scale-type quantities having specific forms. The former $F(\Pi_1, \Pi_2, ..., \Pi_{n-w}) = 0$ is called an "*ensemble*" and the latter $\Pi = \rho(x_1, x_2, x_3, ..., x_n)$ "*regime*"s.

Another constraint named "*identity constraint*" is also used to narrow down the candidate formulae [10]. The basic principle of the identity constraints comes by answering the question that "*what is the relation among Θ_h, Θ_i and Θ_j, if $\Theta_i = f_{\Theta_j}(\Theta_h)$ and $\Theta_j = f_{\Theta_i}(\Theta_h)$ are known?*" For example, if $a(\Theta_j)\Theta_h + \Theta_i = b(\Theta_j)$ and $a(\Theta_i)\Theta_h + \Theta_j = b(\Theta_i)$ are given, the following identity equation is obtained by solving each for Θ_h.

$$\Theta_h \equiv -\frac{\Theta_i}{a(\Theta_j)} + \frac{b(\Theta_j)}{a(\Theta_j)} \equiv -\frac{\Theta_j}{a(\Theta_i)} + \frac{b(\Theta_i)}{a(\Theta_i)}$$

It is easy to prove that the admissible relation among the three is as follows.

$$\Theta_h + \alpha_1\Theta_i\Theta_j + \beta_1\Theta_i + \alpha_2\Theta_j + \beta_2 = 0 \tag{5}$$

The algorithm of SDS is outlined in Fig. 3. In (S1-1), SDS searches bi-variate relations having the linear form in IQ through data fitting. Similar bi-variate equation fitting to the data is applied in (S2-1) and (S2-3) where the admissible equations are power product form and logarithmic form respectively. If this test is passed, the pair of quantities is judged to have the admissible relation of "*Extended Product Theorem.*"

In (S1-2), triplet consistency tests are applied to every triplet of equations in IE. Given a triplet of the linear form equations in IE,

$$\overline{a}_{xy}x + y = b_{xy}, \overline{a}_{yz}y + z = b_{yz}, \overline{a}_{xz}x + z = b_{xz}, \tag{6}$$

the following condition must be met for the three equations to be consistent.

$$\overline{a}_{xz} = -\overline{a}_{yz}\overline{a}_{xy} \tag{7}$$

This condition is used to check if the triplet of quantities belong to an identical regime. SDS applies this test to every triplet of equations in IE, and searches every maximal convex set

MCS where each triplet of equations among the quantities in this set has passed the test. Each MCS is considered to be the linear part of the regime in the formulae given in "*Extended Product Theorem.*" The similar test is applied to the quantities in RE in (S2-2).

Once all regimes are identified, new terms are generated in (S3-1) by merging these regimes in preparation to compose the ensemble equation. SDS searches bi-variate relations between two regimes Πs having one of the formulae specified in the equation set CE. The repertoire in CE governs the ability of the equation formulae search in SDS. Currently, only the two simple formulae of power product form and linear form are given in CE. Nevertheless, SDS performs very well in search for the ensemble equation. When one of the relations specified in CE is found, the pair of the regime Πs is merged into a new term. This procedure is repeated in couple for both product and linear forms until no new term generation becomes possible.

In (S3-2), the identity constraints are applied for further merging terms. The bi-variate least square fitting of the identity constraint such as Eq.(5) is applied to AQ. If all the coefficients except one are independent in a relation, the relation is solved for the unique dependent coefficient, and the coefficient is set to be the merged term of the relation. If all coefficients are independent in a relation, the relation is the ensemble equation. If such ensemble equation is not found, SDS goes back to the (S3-1) for further search.

4 Implementation of SDS2

The major function of SFF is to derive the structural canonical form of the simultaneous equations representing an objective process. However, SDS to discover a complete equation can not directly accept the knowledge of the structural canonical form for the discovery. Accordingly, some additional process to provide information acceptable for SDS is required to consistently implement the two parts into SDS2. First, the problem to derive quantitative knowledge of the simultaneous equations must be decomposed into subproblems to derive each equation individually. For the purpose, an algorithm to decompose the entire problem into such small problems is implemented. The values of the quantities within each independent component DE_i of a complete subset CE_i are mutually constrained, and have the order $\delta m_i = |DQ_i| - \delta n_i$ degree of freedom. Accordingly, the constraints within the independent component disable the bi-variate tests among the quantities of an equation in the structural canonical form, if the order δn_i is more than one. However, this difficulty is removed if the $(\delta n_i - 1)$ quantities are eliminated by the substitutiion of the other $(\delta n_i - 1)$ equations within the independent component. The reduction of the number of quantities by $(\delta n_i - 1)$ in each equation enables to control each quantities as if it is in a complete equation. This elimination of quantities is essential to enable the application of SDS which uses the bi-variate test. The reduction of quantities in equations provides further advantage, since the required amount of computaion in the equation search depends on the number of quantities. In addition, the smaller degree of freedom of the objective equation in the search introduces more robustness against the noise in the data and the numerical error in data fitting. The algorithm for the problem decomposition of SSF which minimizes the number of quantities involved in each equation is given in Fig. 4. This algorithm uses the list of the complete subsets and their order resulted in the algorithm of Fig.2. The quantities involved in each equation are eliminated by the equations in the other complete subset in (S2). In the next (S3), the quantities involved in each equation are eliminated by the other equation within the same complete subset, if the order of the subset is more than one. The quantities to be eliminated in (S2) and (S3) are selected by lexicographical order in the current SSF. This selection can be more tuned up based on the information of the sensitivity to noise and error of each quantities in the future.

Another role of SSF for the equation discovery system is to teach how to control the quantities in the bi-variate experiments. The convntional SDS just tries to fix the values of all quantities except two during the bi-variate tests. However, such control of the objective process is impossible in case of the simultaneous equation system. SDS must be taught the quantities to

Given a set of interval scale quantities, IQ, a set of ratio scale quantities, RQ, and a set of absolute scale quantities, AQ,

(S1-1) Apply bi-variate test for an admissible linear equation of interval scale to every pair of quantities in IQ. Store the resultant bi-variate equations accepted by the tests into an equation set IE and the others not accepted into an equation set NIE.

(S1-2) Apply triplet test to every triplet of associated bi-variate equations in IE. Derive all maximal convex sets MCSs for the accepted triplets, and compose all bi-variate equations into a multi-variate equation in each MCS. Define each multi-variate equation as a term. Replace the merged terms by the generated terms of the multi-variate equations in IQ. Let $RQ = RQ + IQ$.

(S2-1) Apply bi-variate test for an admissible equation of ratio scale to every pair of quantities in RQ. Store the resultant bi-variate equations accepted by the tests into an equation set RE and the others not accepted into an equation set NRE.

(S2-2) Apply triplet test to every triplet of associated bi-variate equations in RE. Derive all maximal convex sets for the accepted triplets, and compose all bi-variate equations into a multi-variate equation in each maximal convex set. Define each multi-variate equation as a term. Replace the merged quantities by the generated terms in RQ.

(S2-3) Apply bi-variate test for an admissible logarithmic equation between the linear forms of interval scale-type quantities and the other terms in RQ. Replace the terms in the resultant bi-variate equations accepted in the tests by the generated terms in RQ.

(S3) Let $AQ = AQ + RQ$. Given candidate formulae set CE, repeat steps (2-1) and (2-2) until no more new term become generated.

(S3-1) Apply bi-variate test of a formula in CE to every pair of the terms in AQ, and store them to AE. Merge every group of terms into a unique term respectively based on the result of the bi-variate test, if this is possible. Replace the merged terms with the generated terms of multi-variate equations in AQ.

(S3-2) Apply identity constraints test to every bi-variate equation in AE. Merge every group of terms into a unique term respectively based on the result of the identity constraints test, if they are possible. Replace the merged terms with the generated terms of multi-variate equations in AQ. Go back to step (2-1).

The candidate models of the objective system are derived by composing the terms in AQ.

Figure 3: Outline of SDS algorithm

(S1) Let DE, DQ and N be the lists obtained in the algorithm of Fig.2.

(S2) For $i = 1$ to $|DE|$ {
For $j = 1$ to $|DE|$ where $j \neq i$ {
If $DE_i \supset DE_j$ where $DE_i, DE_j \in DE$ {
$DE_i = DE_i - DQ'_j$, where DQ'_j is arbitrally, and
$DQ'_j \subset DQ_j \in DQ$ and $|DQ'_j| = \delta n_j$.}}}

(S3) For $i = 1$ to $|DE|$ {
For $j = 1$ to δn_i {
$DE_{ij} = DE_i - DQ_{ij}$, where DQ_{ij} is arbitrally, and
$DQ_{ij} \subset DQ_i \in DQ$ and $|DQ_{ij}| = \delta n_i - 1$.}}

(S4) Every DE_{ij} shows the list of quantities contained in a transformed equation.

Figure 4: Algorithm for minimization.

control and the quantities determined in the process to appropriately arrange the experiments. SSF derives the information by applying a constraint propagation method to the knowledge of the structural canonical form. The algorithm is basically the same with the causal ordering [7].

5 Evaluation of SDS2

SDS2 has been implemented using a numerical processing shell named MATLAB [14]. The performance of SDS2 has been evaluated in terms of the validity of its results, the computational complexity and the robustness against noise through some examples including fairly large scale processes. The objective processes are provided by simulation.

The examples we applied are the following four.

(1) Two parallel resistances and a battery
This is depicted in Fig.1, and has been already explained in the previous sections. Its model consists of 4 equations and 7 quantities as shown in Eqs.1.

(2) Heat conduction at walls of holes
This is a heat conduction preoblem. Given a large solid material having two vertical holes, gas goes into those holes, and condensed to its liquid phase while flowing in the holes by providing its heat energy to the walls of the holes. In these holes, the heat conduction process are represented by 8 equations involving 17 quantities[15].

(3) A circuit of photo-meter
This is a circuit of photo-meter to measure the rate of increase of photo intensity within a time period. The model of this system is represented by 14 equations involving 22 quantities.

(4) Reactor core of power plant
This is a simplifeid nuclear reacotr core model. Nuclear fission reaction process, heat removal of nuclear fuel, and heat and mass balance of reactor coolant are considered. This model involves 24 equations and 60 quantities.

Table 1 is the summary of the specifications of each problem size, complexity and robustness against noise. T_{scf} shows strong dependency on the parameter m and n, i.e., the size of the problem. This is natural, since the algorithm to derive structural canonical forms is NP-hard to the size. In contrast, HM T_{min} shows very slight dependency to the size of the problem, and T_{min} shows very slight dependency on the size of the problem, and the absolute value of the required time is negligible. This observation is also highly consistent with the theoretical view that its complexity should be only $O(n^2)$. The total time T_{tl} does not seem to strongly depend on the size of the problem. This consequence is also very natural, because SDS handles

Table 1: Statistics on complexity and robustness

Ex.	m	n	av	T_{scf}	T_{min}	T_{tl}	T_{av}	NL
(1)	4	7	2.5	3	0.00	206	52	35
(2)	8	17	3.9	1035	0.05	725	91	29
(3)	14	22	2.6	1201	0.05	773	55	31
(4)	26	60	4.0	42395	0.11	3315	128	26

m: number of equation, n: number of quantities, av: average number of quantities/equation, T_{scf}: CPU time (sec) to derive structural canonical form, T_{min}: CPU time to derive minimum quantities form, T_{tl}: CPU time to derive all equations by SDS, T_{av}: average CPU time per equation by SDS, NL: limitation of % noise level of SDS.

each equation separately. The required time of SDS should be proportional to the number of equations in the model. Instead, the efficiency of the SDS more sensitively depends on the average number of quantities involved in each equation. This tendency becomes clearer by comparing T_{av} with av. The complexity of SDS is known to be around $O(n^2)$.

The last column of Table 1 shows the influence of the noise to the result of SDS2, where Gaussian noise is artificially introduced to the measurements. The noise does not affect the computation time in principle. The result showed that a maximum of 25-35% relative noise amplitude to the absolute value of each quantity was acceptable under the condition that 8 times per 10 trials of SDS2 successfully give the correct structure and coefficients of all equations with statistically acceptable errors. The noise sensitivity dose not increase significantly, because SSF focuses on a complete subset which is a small part of the entire system. Similar discussion holds for SDS. The robustness of SDS2 against the noise is sufficient for practical application.

Finally, the validity of the results are checked. In the example (1), SSF derived the expected structural canonical form. Then SSF gave the following form of minimum number of quantities to SDS. Here, each equation is represented by a set of quantities involved in the equation.

$$\{V_e, R_1, I_1\},\ \{V_e, R_2, I_2\},\ \{V_e, V_1\},\ \{V_e, V_2\} \tag{8}$$

As a result, SDS derived the following answer.

$$V_e = I_1 R_1\ [1], V_e = I_2 R_2\ [2], V_e = V_1\ [3] \text{ and } V_e = V_2\ [4], \tag{9}$$

This is equivalent to Eq.(1) not only in the sense of the invariance theorem but also the quantitativeness. Similarly the original equations could be reconstructed in the other examples, and they have been confirmed to be equivalent to the original in the sense of the invariant theorem and quantitativeness.

6 Discussion and Conclusion

As mentioned in the introduction, the conventional equation discovery systems can derive only one or a few complete equation(s) yet with high computational complexity. The research presented here characterized under-constrained simultaneous equations in terms of complete subsets, and provided an algorithm to derive their structure through experiments. In addition, the constraints of scale-type and identity are investigated to be applied to the discovery of each complete equation. These principles studied in this paper provide an effective measure to overcome these conventional limitations.

SSF is a generic tool which can be combined with any conventional equation discovery systems not limited to SDS. Moreover, the principle of SSF can be applied in a more generic

manner not only to the continous processes but also to some discrete systems as far as the systems have structures to propagate states through simultaneous constraints. Main features of SDS are its low complexity, robustness, scalability and wide applicability to the practical problems. The performance of SDS2, an integrated system of these two components: SSF and SDS, was shown convincing by applying to examples of fairly large size.

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