Conditions of Law Equations and the Approach of their Discovery

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Abstract— **This paper discusses the criteria to judge if a given equation represents a set of first principle-based laws or a superficial relation. Based on the criteria, the approach of scientific discovery to automatically discover law equations from data is presented. The state of the art of the scientific law equation discovery has remained to derive candidate law equations without taking into account the criteria of generic mathematical admissibility, and thus many superficial relations can be resulted under the high computational complexity. The principles and the approach presented in this paper overcome these drawbacks. The performance of the presented approach is demonstrated and evaluated through some applications to physics and sociology, and their abilities to derive candidate law equations with high confidence and high efficiency have been confirmed.**

Keywords— **Scientific Discovery, Law Equation, Scale-types.**

I. Introduction

Finding regularities in the data is one of the most major ability of the human intelligence and one of the most major scopes targeted in the artificial intelligence research. Such typical and challenging task is inducing quantitative formulae of scientific laws from measurement data. Langley and others' BACON [1] is the most well known pioneering work to discover a complete equation representing scientific laws governing an objective phenomenon under experimental observations. FAHRENHEIT [2], ABACUS [3], etc. are the successors of BACON that use basically similar algorithms. However, a drawback of the BACON family, that is their low likelihood of the discovered equations being the first principle underlying the objective phenomenon, is reported [4].

To discover the first principle based law equations, some systems, *e.g.*, COPER [5] and the later version of ABACUS, utilize the information of the unit dimensions of quantities to prune the meaningless terms. The basic principle of the pruning is the dimensional homogeneity of units among terms appearing in the equation where the unit dimension of mutually additive terms must be homogeneous. However, the constraint of the dimensional homogeneity is merely a part of the conditions for the first principle based law equations as shown later, and does not provide complete set of solutions. In addition, the application of this approach is limited only to the case that the unit dimension of each quantity in the data is clear. Some extra drawbacks of the aforementioned approaches exist. The data for the discovery must be acquired under experimental observation where the values of some quantities representing the objective phenomenon are observed for various process states by controlling the values of the other relevant quantities.

To alleviate these limitations, the conditions of the first principle based law equations are investigated first. Subsequently, novel principles on scale-type constraints and equation structures to discover the first principle based law equation are shown. Finally, two scientific law discovery systems named "*SDS (Smart Discovery System)*" [6] and its extended version "*Extended SDS*" [7] are explained. SDS is for the experimental environment based on the above principles. Extended SDS is applicable to "*passively observed data*" where any controllable parameters do not exist in the objective phenomenon. The performance of the systems is demonstrated through some applications to physics and sociology domains.

II. Criteria of Law Equations

Various relations among objects, events and/or quantity values are observed in natural and social phenomena. Scientists call the relation as a "law" if it is commonly observed over the wide range of the phenomena in a domain. When the relation of the law can be represented in form of mathematical formulae constraining the values of some quantities characterizing the phenomena, the relation is called "*law equations*". In popular understanding, the relations of the laws and the law equations are considered to be objective in the sense that they are embedded in the phenomena independent of our processes of observation, experiment and interpretation.

However, the definition of the laws and the law equations must be more carefully investigated. For example, given the enforced turbulence flow in a circular pipe, the heat transfer phenomenon from the flow liquid to the pipe wall is represented by the following Dittus-Boelter equation which is well known in thermo-hydrorics domain.

$$Nu = 0.023Re^{0.8}Pr^{0.4}, \quad (1)$$

where $Nu = hd/\lambda$, $Re = \rho ud/\eta$, and $Pr = \eta c_p/\lambda$. $h[W/(m^2 \cdot {}^\circ K)]$ is the coefficient of the heat transfer rate between the liquid and the wall, $d[m]$ the diameter of the circular pipe, $\lambda[W/(m \cdot {}^\circ K)]$, $\rho[kg/m^3]$, $u[m/s]$, $\eta[Pa \cdot s]$, $c_p[J/(kg \cdot {}^\circ K)]$ the heat conductance, density, velocity, viscosity and specific heat of the liquid under a constant pressure respectively [8]. This relation stands objectively independent of our interpretation, and holds for the enforced turbulence flow in a circular pipe in most cases. However, the scientists and the engineers in the thermo-hydrorics domain call this relation as an "*experimental equation*" but not a "*law equation*". On the other hand, the gravity force $F[kg{\cdot}m/s^2]$ interacting between two mass points $M_1[kg]$ and $M_2[kg]$ is represented by the following relation when their interval distance is $R[m]$.

$$F = G\frac{M_1 M_2}{R^2}, \quad (2)$$

where $G[m^3/(kg{\cdot}s^2)]$ is the gravity constant. While this equation is also objective and experimentally obtained similar to the Dittus-Boelter equation, this is called as the "*law equation*" of gravity. Some researchers may claim that this difference is because the former merely represents the relation pretended by the combination of various mechanisms while the latter is the relation representing an elementary mechanism. However, any physical evidence that the law of gravity is elementary has not been obtained yet [9].

The objectiveness of the relations is not sufficient to understand the phenomena. Their representation must be consistent with the assumptions and the operations applied in their discovery processes. Accordingly, the criteria of the laws and law equations can be derived by mathematically characterizing the assumptions and the operations involved in these processes. The research on the criteria of the law equations is not widely seen in the history of science. A popular interpretation is that the law equations are merely empirical relations which are widely known in a research domain and given specific names in the history of the domain. On the other hand, some major scientists have made efforts to establish the definitions and the conditions of law equations based on the axiomatic approaches. Probably, its complete axiomatization without any exception may be difficult since some relations might be named as laws in purely empirical manners. However, the clarification of its criteria is considered to be highly important to give a firm basis of the science. Some of the important conditions on the scientific proposition are given by Descartes. They are clarity, distinctness, soundness and consistency in the deduction of the proposition [10], and these conditions should be also taken into account to clarify the criteria of the scientific law equations. Newton also proposed some conditions of the law equations [11]. The first condition is the objectiveness where the relation reflects only the causal assumptions of the nature while excluding any human's mental effects, the second the parsimony of the causal assumptions supporting the relation, the third the generality where the relation holds over the various phenomena in a domain and the forth the soundness where the relation is not violated by any experimental result performed under the environment following the causal assumptions. Similarly, Simon also claimed the importance of the parsimony of the law description [12]. In the modern physics, the importance of the mathematical admissibility of the relation formulae under the nature of the time and the space became to be stressed by some major physicists including Feynman [9].

We introduce the following definitions and propositions associated with the criteria of the law equations based on the above claims.

Definition 1 (A Scientific Region) A scientific region T is represented by the following quadruplet.

$T = < S, A, L, P >$
where
$S = \{s_h | s_h \text{ is a rule in syntax}, h = 1, ..., p\}$,
$A = \{a_i | a_i \text{ is an axiom in semantics}, i = 1, ..., q\}$,
$L = \{\ell_j | \ell_j \text{ is a postulate in semantics}, j = 1, ..., r\}$,
$P = \{o_k | o_k \text{ is an objective phenomenon}, k = 1, ..., s\}$.

S is the syntax of T, and for example its elements are the coordinate system, the definitions of quantities such as velocity and energy and the definitions of the algebraic operators in physics. The axioms in A are the set of the mathematical relations independent of objective phenomena, for example, the relations of distances among points in an Euclidean space. A postulate $\ell_j (\in L)$ is a law equation where its validity is empirically believed under some conditions which will be described later. An example is the aforementioned law of gravity in physics. A and L give the semantics of T. In addition, the definition of T involves a set of objective phenomena P which is analyzed in the scientific domain, since the scientific domain is established for the purpose to study some limited part of the universe. In other words, S, A and L must be valid within the analysis of P, and hence each ℓ_j is requested to satisfy the conditions of the law equations for P but not requested outside of P. Moreover, an ℓ_j is used in the analysis of a part of P but not necessarily used for all of P. For example, the law of gravity is not necessarily used in the analysis of a spring behavior.

Definition 2 (Objective Phenomena of a Relation) Given a mathematical relation e, if all quantities in e appear in the description of an phenomenon as mutually relevant quantities, the phenomenon is called an "*objective phenomenon of e*". A subset of P, in which the phenomena are the objective of e, is called "*the set of the objective phenomena of e*" $P_e (\subseteq P)$.
For example, the heat transfer from the flow liquid to the circular pipe wall for the enforced turbulence flow is an objective phenomenon of the Dittus-Boelter equation since it is represented by Nu, Re and Pr. Also, a system described by two mass points M_1 and M_2 having an interval distance R and the force F between the points is an objective phenomenon of the law of gravity.

Definition 3 (Satisfaction and Consistency of a Relation) Given a mathematical relation e and its objective phenomenon, if the phenomenon is explicitly constrained by e, e is said to be "*satisfactory*" in the phenomenon. On the other hand, if the phenomenon does not explicitly violate e, e is said to be "*consistent*" with the phenomenon.
When we consider the kinematic momentum conservation in the collision of two mass points, if the mass points are very heavy, this phenomenon is analyzed under the requirement that the law of gravity should be satisfactory. Oth-

erwise, the law of gravity is ignored. But, it should be consistent in both cases.

Based on these definitions and the aforementioned claims of some major scientists, the criteria of a relation e to be a law equation are described as follows.

(1) **Objectiveness**: All quantities appearing in e are observable directly and/or indirectly in the phenomena in P_e.

(2) **Generality**: The satisfaction of e is widely identified in the test on the phenomena included in P_e.

(3) **Reproducibility**: For every phenomenon in P_e, the identical result on the satisfaction and the consistency is identified in repeated tests.

(4) **Soundness**: The consistency of e is identified in the test on every phenomenon in P_e.

(5) **Parsimony**: e includes the least number of quantities to characterize the phenomena in P_e.

Here, the "*test*" is an experiment or an observation, and the "*identification*" is to confirm a fact in the test while considering the uncertainty and/or the accuracy of the test. Though the objectiveness and the generality include the criteria of (3),(4) and (5) in wider sense, each criterion is more specifically defined in this literature to reduce their ambiguity.

The aforementioned Dittus-Boelter equation Eq.(1) including the quantities of Nu, Re and Pr represents the heat transfer phenomenon related with the enforced turbulence flow which belongs to the thermo-hydrorics. The set of the objective phenomena of the thermo-hydrorics P includes all phenomena over all value ranges of Nu, Re and Pr. Thus, according to the definition 2, P_e of the Dittus-Boelter equation is the set of all phenomena represented by Nu, Re and Pr in P. This equation meets the criterion of the objectiveness because Nu, Re and Pr are observable through some experiments. It is general over various enforced turbulence flows in circular pipes and reproducible for the repetition of the tests. It also has a parsimonious shape. However, this equation is not sound in P_e, because it stands for only the value ranges of $10^4 \leq Re \leq 10^5$ and $1 \leq Pr \leq 10$, and is explicitly violated outside of these ranges. In this regard, this equation is not a law equation. On the other hand, P of the classical mechanics includes the phenomena represented by mass, distance and force, and thus P_e of Eq.(2) is the set of all phenomena represented in some value ranges of these quantities. This equation also meets the criteria of objectiveness, generality, reproducibility and parsimony in P_e. Furthermore, as any phenomena in P_e do not violate this relation, it is sound.

However, an extra criterion is requested for the law equation according to the definition 1.

(6) **Mathematical Admissibility**: e follows the syntax S and the axioms of the semantics A.

The admissibility of e is not limited to the constraints of some fundamental notions in mathematics such as arithmetic operations but also the unit dimensional homogeneity [13],[14] and the scale-type constraints as described later. For example, Eq.(2) satisfies the dimensional homogeneity because its lhs and rhs have identical unit dimension $[kg{\cdot}m/s^2]$.

III. Scale-type Constraints

The criteria of (1)—(4) are checked through actual experiments and/or observations, if the processes of the experiments and/or the observations are well-defined. In contrast, the criteria of (5) and (6) are the conditions on the shape of the equation formulae and not directly dependent of the experiments and/or the observations. For the criterion of (5) parsimony, the appropriate description of the relation under the trade off between the accuracy and the complexity of the relation has been extensively studied, and some systematic criteria such as AIC in statistics [15] and MDL in information theory [16] are widely known. On the criterion of (6) mathematical admissibility, the constraints of some fundamental notions in mathematics such as arithmetic operations are very weak to constrain the shape of the relation formulae. A stronger constraint is the aforementioned analysis on the unit dimension which is applicable when the unit of each quantity is clear in the relation. However, the units of many major quantities in the domains of psychology, sociology, economics and biology are unclear since the detailed procedures to measure the quantities are not well established. Therefore, generic and strong constraints of the mathematical admissibility must be explored. The value of a quantity is obtained through a measurement in most of the scientific domains, and some features of the quantity are characterized by the measurement process. Though the unit dimension is an example of such features, a more generic feature is "scale-types." Stevens defined the measurement process as "*the assignment of numerals to object or events according to some rules*," and claimed that the rule set defines the "*scale-type*" of the measured quantity. He categorized the scale-types into "*nominal*", "*ordinary*", "*interval*" and "*ratio*" scales [17]. In the later study, another scale-type called absolute scale is added. Subsequently, Krantz et al. axiomatized the measurement processes and the associated scale-types [18]. In the meantime, Luce claimed that the basic formula of the functional relation among quantities of ratio and interval scales can be determined by their scale-type [19]. In this section, the theory of the scale-types is reviewed.

Among the scale-types, the scale-types of the quantitative quantities are interval, ratio and absolute scales. 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. Its operation rule is "*determination of equality of intervals or differences*", and its admissible unit conversion "$x' = kx + c$" preserves the structure of "*Generic linear group.*" Examples of the ratio scale quantities are physical mass and absolute temperature where each has an absolute zero point. Its operation rule is "*determination of equality of ratios*," and its admissible unit conversion follows "*Similarity group*: $x' = kx$." Examples of the absolute scale quantities are dimensionless quantities such as Nu, Re and Pr in Eq.(1). It follows the rule of "*determination of equality of absolute value*", and "*Identity group*: $x' = x$."

Luce claimed that the basic formula of the functional relation among two quantities of ratio and interval scales can be determined by their scale-type features, if the two quantities have direct dependency without being coupled through any dimensionless quantities [19]. Under this condition, some unit dimensions are shared between the two quantities, and consequently the unit change of a quantity affects the value of the other quantity. Suppose x_i and x_j are both ratio scale quantities, and x_i is defined by x_j through a logarithmic functional relation $x_i = u(x_j)$, *i.e.*, $x_i = \log x_j$. We multiply a positive constant k to x_j, *i.e.*, a change of unit, without violating the group structure of the ratio scale quantity x_j, then this leads $u(kx_j) = \log k + \log x_j$. This fact causes the shift of the origin of x_i by $\log k$, and violates the group structure of x_i which is the ratio scale quantity. Hence, the direct functional relation from x_j to x_i must not be logarithmic. As the admissible transformations of x_i and x_j in their group structures are $x'_j = kx_j$ and $x'_i = Kx_i$ respectively, the generic formula of $x_i = u(x_j)$ must satisfy the invariant condition of $x'_i = u(x'_j) \leftrightarrow Kx_i = u(kx_j)$ under the unit conversion. The factor K of the changed unit of x_i depends on k, but it shall not depend upon x_j, so we denote it by $K(k)$. Consequently, we obtain the following constraints on the continuous function $u(x_j)$.

$$u(kx_j) = K(k)u(x_j),$$

where $k > 0$ and $K(k) > 0$ as these are the factors of the unit change. The constraints for all combinations of the scale types are summarized in Table I [19]. Luce derived each solution of $u(x_j)$ under the condition of $x_j \geq 0$ and $u(x_j) \geq 0$. We have extended his theory to cover the negative values of x and $u(x_j)$ [20]. The generic solution of $u(x_j)$ in each case is summarized in Table II. The impossibility of the definition of a ratio scale from an interval scale is because the ratio scale involves the information of an absolute origin, but the interval scale does not.

IV. Structure of Law Equations

In the unit dimensional analysis, the following theorem has been provided independently of the aforementioned study on scale-types [13].

Theorem 1 (Product Theorem) Given some ratio scale quantities $x, y, ...$, a derivative quantity f is related by the following formula.

$$f = Cx^a y^b z^c ...$$

where $C, a, b, c, ...$ are constants.
By introducing the consequences of Luce to this theorem, we extended the theorem to the case where the quantities of ratio, interval and absolute scales are included in the formula.

Theorem 2 (Extended Product Theorem) Given a set of ratio scale quantities R and a set of interval scale quantities I, a derivative quantity Π is related with each $x_i \in R \cup I$ through one of the following formulae.

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

$$\Pi = \sum_{x_i \in R} a_i \log|x_i| + \sum_{I_k \in C_{\bar{g}}} a_k \log(\sum_{x_j \in I_k} b_{kj}|x_j| + c_k)$$

$$+ \sum_{x_\ell \in I_g} b_{g\ell}|x_\ell| + c_g,$$

where R or I can be empty, and C is a covering of I, $C_{\bar{g}}$ a covering of $I - I_g$ ($I_g \subseteq I$). Π can be any of interval, ratio and absolute scale, and each coefficient is constant.
When the argument quantities appearing in a law equation are ratio scale and/or interval scale, the relation among the quantities sharing arbitrary unit dimensions has one of the above formulae.

Together with the above Product Theorem, another major theorem of the unit dimensional analysis characterizes the structure of admissible law equations [14].

Theorem 3 (Buckingham Π-theorem) Given a complete equation $\phi(x, y, ...) = 0$, if every argument of this equation is ratio scale, then the equation can be rewritten in the following form.

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

where n is the number of the arguments of ϕ, r is the number of the basic unit contained in $x, y, ...$, and Π_i is absolute scale for all i.
A basic unit is the unit dimension which defines the scaling independent of the other unit in ϕ as length $[L]$, mass $[M]$ and time $[T]$. Each $\rho_i(\Pi_i, x, y, ...) = 0$ defining Π_i is called a "*regime*" and $F(\Pi_1, \Pi_2, ..., \Pi_{n-r}) = 0$ an "*ensemble*" in the unit dimensional analysis. Because all arguments of $F = 0$ are absolute scale, *i.e.*, dimensionless, the shape of the formula does not constrained by the theorem 1 and 2, and its arbitrary formula is admissible in terms of the scale-type.

We also extended this theorem to include the interval, ratio and absolute scale quantities in the argument.

Theorem 4 (Extended Buckingham Π-theorem) Given a complete equation $\phi(x, y, z, ...) = 0$, if every argument of this equation is either of interval, ratio and absolute scales, then the equation can be rewritten in the following form.

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

where n is the number of the arguments of ϕ, r and s are the numbers of the basic unit and the basic origin contained in $x, y, ...$, and Π_i is absolute scale for all i and represented by the formulae of the *regime* defined by Extended Product Theorem.
Here, the basic origin is the origin which is artificially chosen in the measurement of an interval scale quantity, for example, the origin of temperature in Celsius defined as

TABLE I

CONSTRAINTS ON FUNCTIONAL RELATIONS UNDER SCALE-TYPE CHARACTERISTICS.

C_n No.	SCALE TYPES: INDEPENDENT VARIABLE x_j	SCALE TYPES: DEPENDENT (DEFINED) VARIABLE x_i	CONSTRAINTS*	COMMENTS*
1	RATIO	RATIO	$u(kx_j) = K(k)u(x_j)$	$k > 0, K(k) > 0$
2	RATIO	INTERVAL	$u(kx_j) = K(k)u(x_j) + C(k)$	$k > 0, K(k) > 0$
3	INTERVAL	RATIO	$u(kx_j + c) = K(k, c)u(x_j)$	$k > 0, K(k, c) > 0$
4	INTERVAL	INTERVAL	$u(kx_j + c) = K(k, c)u(x_j) + C(k, c)$	$k > 0, K(k, c) > 0$

*C AND C CAN BE ANY REAL NUMBERS.

TABLE II

THE ADMISSIBLE RELATIONS UNDER SCALE-TYPE CHARACTERISTICS.

Eq. No.	SCALE TYPES: INDEPENDENT VARIABLE x_j	SCALE TYPES: DEPENDENT (DEFINED) VARIABLE x_i	POSSIBLE RELATIONS	COMMENTS*
1	RATIO	RATIO	$x_i = \alpha_* \lvert x_j \rvert^{\beta}$	$\beta/x_j, \beta/x_i$
2.1	RATIO	INTERVAL	$x_i = \alpha \log \lvert x_j \rvert + \beta_*$	α/x_j
2.2			$x_i = \alpha_* \lvert x_j \rvert^{\beta} + \delta$	$\beta/x_j; \beta/x_i; \delta/x_j$
3	INTERVAL	RATIO	IMPOSSIBLE	
3.1			$x_i = \alpha_{*a} e^{\beta x_j}$	β/x_j
3.2			$x_i = \alpha_{*b} \lvert x_j + \delta \rvert^{\beta}$	$\beta/x_j; \beta/x_i; \delta/x_j$
4	INTERVAL	INTERVAL	$x_i = \alpha_* \lvert x_j \rvert + \beta$	β/x_j

1) THE NOTATIONS α_*, β_* ARE α_+, β_+ FOR $x_j \geq 0$ AND α_-, β_- FOR $x_j < 0$, RESPECTIVELY.
2) THE NOTATIONS α_{*a} IS α_+ FOR $x_i \geq 0$ AND α_- FOR $x_i < 0$, RESPECTIVELY.
3) THE NOTATIONS α_{*b} IS α_{++} FOR $x_i \geq 0, x_j - \delta \geq 0$, α_{+-} FOR $x_i \geq 0, x_j - \delta < 0$, α_{-+} FOR $x_i < 0, x_j - \delta \geq 0$, AND α_{--} FOR $x_i < 0, x_j - \delta < 0$, RESPECTIVELY.
4) THE NOTATIONS α/x MEANS "α IS INDEPENDENT OF THE UNIT x".
5) THE RELATIONS IN 3.1 AND 3.2 ARE NOT DERIVED FROM THEIR CONSTRAINTS, BUT ARE INVERSE FUNCTIONS OF 2.1 AND 2.2.

the melting point of water under the standard atmosphere pressure. The formula of the ensemble equation is also arbitrary in this theorem since its all arguments are absolute scale.

The following example of the nuclear decay of a radioactive element demonstrates the theorem 2 and the theorem 4.

$$N = N_0 \exp[-\lambda(t - t_0)] \quad (3)$$

where $t[s]$: time, $t_0[s]$: time origin, $\lambda[s^{-1}]$: decay speed constant, $N[kg]$: current element mass and $N_0[kg]$: original element mass. t and t_0 are interval scale, and λ, N and N_0 are ratio scale. By introducing dimensionless Π_1 and Π_2, the equation can be rewritten as

$$\Pi_1 = \exp(-\Pi_2), \quad (4)$$
$$\Pi_1 = N/N_0, \quad (5)$$
$$\Pi_2 = \lambda(t - t_0), \quad (6)$$

which are an *ensemble* and two *regimes*. The *regimes* (5) and (6) follow the first formula in the theorem 2. The number of the original arguments n is 5. r is equal to 2 because t, t_0 and λ share a basic unit of time $[s]$ and N and N_0 share the basic unit of mass $[kg]$. s is equal to 1 since t and t_0 share a basic origin of time. Thus $n - r - s = 2$ holds, and this satisfies the theorem 4.

As indicated in the above example, the scale-type of measurement quantities strongly constrains the formulae of the law equations. Empirical equations which relate the measurement quantities in arbitrary formulae do not provide excellent knowledge representation for domain experts to understand phenomena.

V. SDS AND EXTENDED SDS

In this section, the algorithms of two scientific discovery systems named "*SDS (Smart Discovery System)*" and "*Extended SDS*" are described. The former discovers law equations under the experimental environment, and the latter discovers under passive observation where any active control of parameters on the objective phenomena is now allowed. Prior to the explanation of each scientific law equation discovery system, the conditions required to discover law equations following the aforementioned criteria are discussed.

A. Required Conditions

SDS has to check the criteria of objectiveness, generality, reproducibility, soundness, parsimony and mathematical admissibility through the experiments on the objective phenomena. Strictly speaking, the verifications of the generality and the soundness are very hard since they require the experimental knowledge on various phenomena. However, these can be checked if we relax the requirements to limit the verification within a given set of the objective phenomena. Under this premise, the following procedures to check the criteria are introduced into SDS and Extended SDS.

1. **Objectiveness**: An equation is sought to relate some quantities directly or indirectly observed in the objective phenomena.
2. **Generality**: An equation is sought to explain all behaviors shown by the combinations of the values of some quantities in the objective phenomena.
3. **Reproducibility**: An equation is sought to give identical result on the consistency with each behavior in the repetition of the experiments on the objective phenomena.
4. **Soundness**: An equation is sought not to contradict with all behaviors in the objective phenomena.
5. **Parsimony**: An equation is sought to relate less number of quantities observed in the objective phenomena.
6. **Mathematical Admissibility**: An equation is sought to follow the formulae specified in the theorems 2 and 4.

The objectiveness is easily ensured if the equation is searched within the quantities given in the observed data. In addition, the generality is subsumed by the soundness due to the aforementioned relaxation of the requirement to limit the phenomena for the verification. An important point to perform these procedures is to establish a method to check if an equation holds for all behaviors which can be occurred in the objective phenomena. A natural approach is to collect all possible combinations of the values of the quantities and to fit the various candidate equations to the collected data. However, this generate and test approach faces the combinatorial explosion in the data collection and the candidate equation generation. To avoid this difficulty, we introduce the following conditions for SDS under experimental environment.

(a) The objective phenomena are represented by a complete equation.

(b) The objective phenomena are static, or the time derivatives of some quantities are directly observable if the phenomena are dynamic.

(c) The scale-types of all quantities needed to represent the objective phenomenon are known.

(d) All quantities except one dependent quantity are controllable at least.

(e) Given a pair of any quantities observed in the objective phenomena, the bi-variate relation on the pair can be identified while fixing the values of the other quantities.

The first and the second conditions are common in BACON family to reduce the search space by searching for every equation separately and limiting the search to snapshot behaviors. The third condition comes from the fact that SDS uses the information of the scale-types of the quantities to

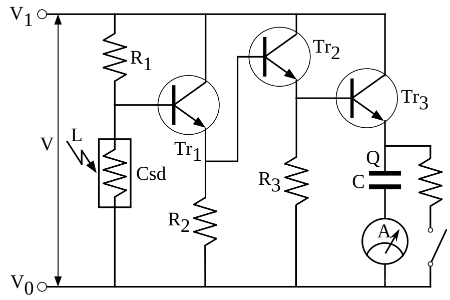

Fig. 1. A circuit of photo-meter

search mathematically admissible equation formulae to relate the quantities. As the scale-types of the measurement quantities are widely known based on the measurement theory [6], this condition does not restrict the applicability of SDS. The last two conditions are to ensure the application of SDS to experimental environment in scientific laboratories. These conditions are also requested in BACON family.

Extended SDS discovers the law equations from the passively observed data, and thus the aforementioned conditions (d) and (e) are not required. Instead, it needs the following condition.

(f) The observed data are uniformly distributed over the possible states of the objective phenomenon.

Violation of the requirement of the uniform distribution over a certain value range of a quantity implies the low observability of the quantity [7],[21]. Any approaches such as the linear system identification and the neural network do not derive valid models under low observability. This limitation is generic, and further discussion on this issue is out of scope of this paper.

B. SDS

If any pair of interval and/or ratio scale quantities $\{x, y\}$ in a given complete equation is to belong to an identical regime, they has to have a relation that follows the Theorem 2. Conversely, SDS searches bi-variate relations in the set of quantities Q where the relations have the following product, linear or logarithmic forms which are deduced from the Theorem 2.

$$x^a y = b, \text{ where } x, y \text{ are ratio scale,} \quad (7)$$

$$ax + y = b, \text{ where } x, y \text{ are interval scale, and} \quad (8)$$

$$a \log x + y = b \text{ or } cx^a + y = b, \quad (9)$$

where x is ratio, and y interval scale.

The value of the constant a in each formula must be independent of any other quantities according to Extended Product Theorem, while the constants b and c are dependent on the other quantities in the regime. SDS applies the least square fitting of these relations to the bi-variate experimental data of x and y that are measured while holding the other quantities constant in Q, and determines the values of coefficients in the bi-variate relations. Subsequently, the judgment is made whether this equation fits the data well enough by some statistical tests. This procedure is called "*bi-variate fitting.*"

This is now demonstrated by an example of a complex system depicted in Fig. 1. This is a circuit of photo-meter to measure the rate of increase of photo intensity within a certain time period. The resistance and switch parallel to the capacitor and the current meter are to reset the operation of this circuit. The actual model of this system is represented by the following complex equation involving 18 quantities.

$$(\frac{R_3 h_{fe_2}}{R_3 h_{fe_2} + h_{ie_2}} \frac{R_2 h_{fe_1}}{R_2 h_{fe_1} + h_{ie_1}} \frac{rL^2}{rL^2 + R_1})(V_1 - V_2) - \frac{Q}{C} - \frac{K h_{ie_3} X}{B h_{fe_3}} = 0. \quad (10)$$

Here, L and r are photo intensity and sensitivity of the Csd device. X, K and B are position of indicator, spring constant and intensity of magnetic field of the current meter respectively. h_{ie_i} is input impedance of the base of the i-th transistor. h_{fe_i} is gain ratio of the currents at the base and the collector of the i-th transistor. The definitions of the other quantities follow the standard symbolic representations of electric circuit. h_{fe_i}s are absolute scale, V_1 and V_2 interval scale, and the rest ratio scale. X is the dependent quantity in this circuit, and the others are independently controllable by the change of boundary conditions and the replacement of devices. SDS requests the bi-variate change of quantities to the experimental environment. When a quantity is dependent (not controllable) during the search process, SDS modifies its request to control the other independent quantity. A simulation based experimental environment was designed and build for the circuit system. $\pm 4\%$ (std.) of relative Gaussian noise was added to both of the control quantity (input) and the measured quantity (output) in every bi-variate fitting. First, SDS set the set of interval scale quantities IQ as $\{V_1, V_2\}$, ratio scale quantities RQ as $\{L, r, R_1, R_2, R_3, h_{ie_1}, h_{ie_2}, h_{ie_3}, Q, C, X, K, B\}$ and absolute scale quantities AQ as $\{h_{fe_1}, h_{fe_2}, h_{fe_3}\}$ based on the input information on scale-types. Next, it performed the bi-variate fitting of a linear form Eq. (8) to the experimental data among the quantities in IQ, and applied the statistical tests. Then, SDS figured out a set consisting of a bi-variate equation $IE = \{\Theta_0 = 1.000V_1 - 1.000V_0\}$ quickly. Subsequently, a product form Eq. (7) among the quantities in $RQ \cup \{\Theta_0\}$ is searched, and applied the statistical tests.

The resultant set of the bi-variate equations RE that passed the tests was as follows.

$$\begin{aligned} RE = & \\ & \{L^{1.999} r = b_1, L^{-1.999} R_1 = b_2, r^{-1.000} R_1 = b_3, \\ & R_2^{-1.000} h_{ie_1} = b_4, R_3^{-1.000} h_{ie_2} = b_5, Q^{-1.000} C = b_6, \\ & h_{ie_3}^{1.000} X = b_7, h_{ie_3}^{1.000} K = b_8, h_{ie_3}^{-1.000} B = b_9, \\ & X^{1.000} K = b_{10}, X^{-0.999} B = b_{11}, K^{-1.000} B = b_{12}.\} \end{aligned}$$

The bi-variate fitting of Eq. (9) for the other pairs across IQ and RQ have also been conducted. But no equations have passed the statistical tests.

In the next step, triplet consistency tests are applied to every triplet of equations in $IE \cup RE$. In case of a triplet of the power form equations, $x^{a_{xy}} y = b_{xy}, y^{a_{yz}} z = b_{yz}, x^{a_{xz}} z = b_{xz}$, by substituting y in the first to y in the second, we obtain $x^{-a_{yz} a_{xy}} z = {b_{xy}}^{-a_{yz}} b_{yz}$. Thus, the following condition must be met.

$$a_{xz} = -a_{yz} a_{xy}.$$

However, if any of the three equations are not correct due to the noise and error of data fitting, this relation may not hold. Thus, a statistical test judges if the three of the equations are mutually consistent in terms of as. For the triplet of the linear form equations, a similar test is applied based on the identical principle. SDS applies this test to every triplet of equations in $IE \cup RE$, and search every maximal convex set MCS where each triplet of equations among the quantities in this set are mutually consistent. The value of each a is evaluated by its average $\overline{a}$ over the equations in the MCS. When the value of $\overline{a}$ is close enough to its nearest integer within its statistical error bound, it is set to the integer value. This operation is based on the observation that the majority of the first principle based equations have integer power coefficients. Finally, the merged quantities are replaced by the term of each equation of the derived regime in $IQ \cup RQ$. In the example in Fig. 1, the final forms of regimes were represented by the merged terms in $IQ \cup RQ$ as follows.

$$\begin{aligned} IQ \cup RQ = & \{\Pi_1 = R_1 r^{-1} L^{-2}, \Pi_2 = h_{ie_1} R_2^{-1}, \Pi_3 = h_{ie_2} \\ & R_3^{-1}, \Pi_4 = h_{ie_3} XKB^{-1}, \Pi_5 = QC^{-1}, \Theta_0 = V_1 - V_0\} \end{aligned}$$

Once all regimes are identified, new terms are further generated by merging these regimes in $IQ \cup RQ \cup AQ$. SDS searches bi-variate relations having one of the formulae $x^a y = b$ (product form) and $ax + y = b$ (linear form) by adopting the least square fitting of these formulae. Then, the statistical tests of the goodness of the fitting are applied. In the example of the circuit, the product form was applied first. They were merged to the following new terms.

$$\begin{aligned} \Theta_1 &= \Pi_1 h_{fe_1} = R_1 r^{-1.0} L^{-2.0} h_{fe_1}, \\ \Theta_2 &= \Pi_2 h_{fe_2} = h_{ie_1} R_2^{-1.0} h_{fe_2}, \\ \Theta_3 &= \Pi_3 h_{fe_3} = h_{ie_2} R_3^{-1.0} h_{fe_3}. \end{aligned}$$

Next, the linear form was tested, then a form was found.

$$\Theta_4 = \Pi_4 + \Pi_5 = h_{ie_3} XKB^{-1.0} + QC^{-1.0}$$

Thus, $IQ \cup RQ \cup AQ$ became as $\{\Theta_0, \Theta_1, \Theta_2, \Theta_3, \Theta_4\}$. Again, by applying the product form, another was newly generated.

$$\Theta_5 = \Theta_0 \Theta_4^{-1.0} = (V_1 - V_0)(h_{ie_3} XKB^{-1.0} + QC^{-1.0})^{-1.0}$$

Thus, $IQ \cup RQ \cup AQ = \{\Theta_1, \Theta_2, \Theta_3, \Theta_5\}$. As no new terms became available, this step was finished.

In the final step, the "*identity constraint*" are applied to further merge terms. 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 relation is deduced.

$$\Theta_h + \alpha_1 \Theta_i \Theta_j + \beta_1 \Theta_i + \alpha_2 \Theta_j + \beta_2 = 0$$

This principle is generalized to various relations among multiple terms. In the example of the circuit, SDS found a set of the bi-variate linear relations on the combinations of $\{\Theta_1, \Theta_5\}, \{\Theta_2, \Theta_5\}$ and $\{\Theta_3, \Theta_5\}$. By applying the identity constraint, the following multi-linear formula has been obtained.

$$\Theta_1\Theta_2\Theta_3 + \Theta_1\Theta_2 + \Theta_2\Theta_3 + \Theta_1\Theta_3 + \Theta_1 + \Theta_2 + \Theta_3 + \Theta_5 + 1 = 0$$

Because every coefficient is independent of any terms, this is considered to be the ensemble equation. The equivalence of this result to Eq. (10) is easily checked by substituting the intermediate terms to this ensemble equation.

Main features of SDS are its low complexity, robustness, scalability and wide applicability. The basic algorithm of SDS consists of two types of procedures. One is the bi-variate fitting for each pair of quantities and terms. The complexity of this procedure is $O(n^2mk)$ where n, m, k are the number of quantities to represent the objective phenomenon, the number of experimental data used for a data fitting and the number of iteration of the data fitting in a bi-variate fitting respectively. Another is the triplet test for each triplet of quantities and terms, where its complexity is $O(n^3)$. m and k usually do not affect the performance of SDS as they are almost independent of the complexity of objective phenomenon. Moreover, the computational cost required in the bi-variate fitting is much larger than the triplet test because the former involves multiple experiments, data sampling, data fitting and some statistical tests, whereas the latter involves the triplet consistency checking among the given coefficients only. Thus, the practical complexity is almost proportional to the second order of n. Table III shows the performance of SDS to discover various physical law equations under simulations. The relative CPU time of SDS normalized by the first case shows that its complexity is nearly proportional to n^2. For reference, the relative CPU time of ABACUS is indicated for the same cases except for the circuit examples of this paper[3]. Though ABACUS applies various heuristics including the information of dimension, its complexity is still non-polynomial. As this feature is shared by BACON family, they can hardly derive the model of the electric circuit of this complexity.

The robustness of SDS against the noisy experimental environment has been also evaluated. The upper limitation of the noise level to obtain the correct result in the cases of more than 80% of 10 trials was investigated for each physical law, and they are indicated in the last column of Table III. The noise levels shown here are the std. of Gaussian noise relative to the real values of quantities, and were added to both controlled (input) quantities and measured (output) quantities at the same time. Thus actual noise level is higher than these levels. The results show the significant robustness of SDS. SDS can provide appropriate results under any practical noise condition.

The low complexity and the high robustness shown here ensure the significant scalability of SDS to engineering problems. Many systems in BACON family adopt generate and test in the search. In contrast, the low complexity of SDS comes from its straightforward algorithm to apply only product and linear forms in polynomial time order in concert with the highly restrictive but domain independent constraints. The robustness of SDS comes from the bi-variate direct fitting to data and the structure of the triplet test. The systems in BACON family repeat formulae fitting to coefficients resulted from the other fitting if it is necessary. This method accumulates the error of data fitting, and derives erroneous results. On the other hand, SDS uses only the bi-variate and direct fitting to the given data, and efficiently composes the result in statistically accurate manner.

TABLE III

STATISTICS ON COMPLEXITY AND ROBUSTNESS

Example	n	TC(S)	TC(A)	NL(S)
Ideal Gas	4	1.00	1.00	±40%
Momentum	8	6.14	22.7	±35%
Coulomb	5	1.63	24.7	±35%
Stoke's	5	1.59	16.3	±35%
Kinetic Energy	8	6.19	285.	±30%
Circuit*1	17	21.6	-	±20%
Circuit*2	18	21.9	-	±20%

n: Number of Quantities, TC(S): Total CPU time of SDS, TC(A): Total CPU Time of ABACUS, NL(S): Limitation of Noise Level of SDS, *1: Case that electronic voltage is represented by a ratio scale V, *2: Case that electronic voltage is represented by two interval scale V_0 and V_1.

C. Extended SDS

As noted in the previous section, the bi-variate fitting requires experimental control of some quantities, and is not applicable to the passive observation environments. To overcome this difficulty, the "*quasi-bi-variate fitting*" procedure depicted in Fig. 2 is used to extract a bi-variate relation between two quantities under the approximated constant values of the other quantities. Let $OBS = \{X_1, X_2, ..., X_n\}$ be a set of observations where each X is a m-dimensional vector of m quantities. The fitting of a candidate bi-variate formula for a pair of two quantities $P_{ij} = \{x_i, x_j\}(\subseteq X)$ is applied to a subset of OBS. This subset OBS_{ijg} is chosen in such a way that every quantity $x_k \in (X - P_{ij})$ takes a value in the vicinity of the value of x_{kg}, where $X_g = \{x_{1g}, x_{2g}, ..., x_{mg}\} \in OBS$ is an arbitrary chosen observation vector. The vicinity of x_{kg} is defined as

$$\Delta x_k = |x_k - x_{kg}| < \epsilon_k.$$

ϵ_k determines the size of the vicinity. This vicinity is indicated by a rectangular cube in the left figure of Fig. 2. Every admissible bi-variate formula is generally represented in the form

$$F_{ij}(P_{ij}, a_{ij}, G_{ij}(X - P_{ij}), H_{ij}(X - P_{ij})) = 0. \qquad (11)$$

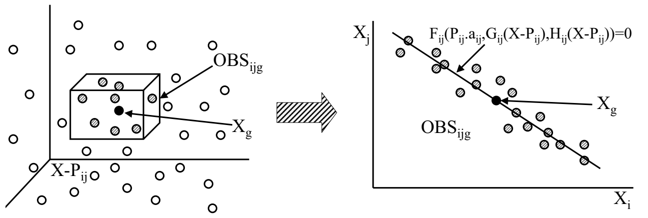

Fig. 2. Outline of quasi-bi-variate fitting

Here, G_{ij} and H_{ij} are dependent on the quantities in $X - P_{ij}$, while a_{ij} remains constant. Given an OBS_{ijg}, if each ϵ_k is moderately small, the values of G_{ij} and H_{ij} become almost constant. The least square fitting of Eq.(11) approximately provides the functional relation within P_{ij} and the coefficient a_{ij} as depicted in the right figure of Fig. 2 while almost excluding the influence of the other dimensions $X - P_{ij}$. The goodness of the fitting is judged by some statistical tests. For the bi-variate relations of the identity constraints, the similar scheme of the quasi-bi-variate fitting is applied.

The proposed method has been applied to a real world problem. The objective of the application is to discover a generic law formula governing the mental preference of people on their houses subject to the cost to buy the house and the social risk at the place of the house. We designed a questionnaire sheet to ask the preference of the house in the trade off between the frequency of huge earthquakes, x_1 (earthquake/year), and the cost to buy, x_2 (\$). These are ratio scale quantities. In the questionnaire, 9 combinations of the cost and the earthquake frequency are presented, and each person chooses its preference from the 7 levels for each combination. We distributed this questionnaire sheet to the people owning their houses in the suburb area of Tokyo, and totally 400 answer sheets are collected back. The answer data has been processed by following the method of successive categories which is widely used in the experimental psychology to compose an interval scale preference index y [22], and $OBS = \{X_1, X_2, ..., X_{400}\}$ where $X_i = [x_{1i}, x_{2i}, y_i]$ is obtained. The expected basic structure of the law equation governing the data is $y = f(x_1, x_2)$. The quasi-bi-variate fitting between x_1 and x_2 was applied, and $x_1 = a(y)x_2^{-0.25}$ have been obtained. Next, the formulae between x_1 and y have been identified as either one of $y = a(x_2)x_1^{-0.23} + b(x_2)$ and $y = 0.62 \log x_1 + b(x_2)$. Similar search has been made for x_2 and y, and, likewise, two candidate equations $y = a(x_1)x_2^{0.026} + b(x_1)$ and $y = 0.34 \log x_2 + b(x_1)$ have been derived. Subsequently, the triplet test among $\{x_1, x_2, y\}$ is conducted, and only the following two candidates have passed the test.

$$y = 0.63 \log x_1 + 0.34 \log x_2 - 2.9 \quad (12)$$

$$y = -0.61 x_1^{-0.23} x_2^{0.026} + 3.2 \quad (13)$$

Though both are admissible as law equations based on the mathematical constraints and the given data, Eq. (12) is preferred as a law equation in terms of the principle of parsimony, because it gives less error for the questionnaire data, and has less number of parameters.

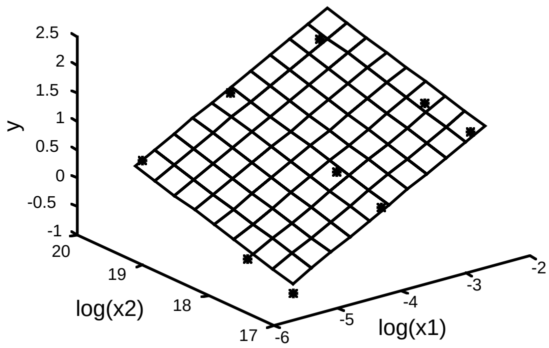

Fig. 3. Plot of Eq.(12)

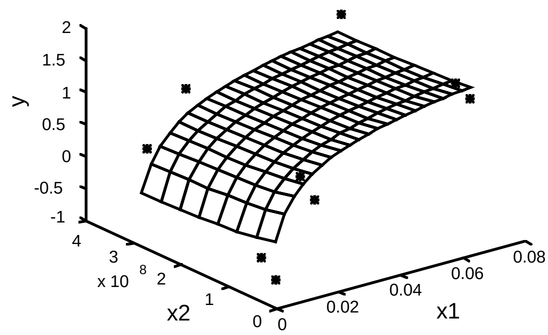

Fig. 4. Plot of Eq.(13)

Figures 3 and 4 shows the plots of the two equation curves together with the average values '■' of the 400 answered preference level y for the 9 cases of the price and the earthquake frequency. The high accuracy of the Eq.(12) is clearly observed in those figures. Eq.(12) can evaluate the subjective preference in the accuracy of almost ± 1 levels of the questionnaire from the values of x_1 and x_2.

VI. Discussion and Conclusion

In this literature, the criteria on the relation among quantities observed in objective phenomena to be a law equation were discussed first. Especially, the criterion of the mathematical admissibility has been analyzed in detail. The definitions of scale-types of quantities and the admissibility conditions on their relations based on the characteristics of the scale-types have been introduced, and the extension of the major theorems in the unit dimensional analysis was shown. Through these analyses, the criteria of the law equation have been clarified. Moreover, the algorithm to discover candidate law equations from measurement data is developed and implemented into programs SDS and Extended SDS based on the above discussion, and its performance evaluation has been conducted in the domains of physics and sociology. In the evaluation, the validity of the presented principles has been confirmed, and the method to systematically discover candidate law equations has been established.

A scientific discovery system called LAGRANGE [23] is applicable to the condition of the passive observation.

It uses the principles of ILP and generate/test. A mutimodal reasoning method proposed by Stolle and Bradley can also automatically construct models of systems under the passive observation through a certain generate/test procedure [24]. Though no equation classes are presumed in these approaches, many spurious solutions can be retained due to the weakness of the modeling heuristics. TETRAD [25] is another system to identify the models of the objective phenomenon from the passive observation. Its basic framework takes the bottom up modeling approach. However, the class of the model formulae is presumed such as linear expressions. In contrast, the method shown in this paper has a strong mathematical background to characterize first principle based model equations. Moreover, it has a powerful applicability to the passive observation data, while maintaining the flexibility of the bottom up modeling approach taken by the conventional scientific discovery systems and the efficiency of the reasoning induced by the scale-type and the identity constraints. The high applicability of this method to various domains including physics, biology, econometrics, sociology etc. is expected.

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