Discovery of Possible Law Formulae Based on Measurement Scale

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Abstract: *We propose a novel approach to automatically discover law formulae of first principles from the measurement data. Our approach lies in between the deductive approaches as represented by dimension-based and symmetry-based reasoning and the empirical approaches as represented by BACON. We try to use the knowledge of the target relation as little as possible, so that it can be applied to various domains which are not limited to physics problem. In spite of its data-driven feature, the formulae obtained by our approach are ensured to represent sound law formulae of first principles similarly to the dimension-based approach. The basic idea is the combined use of deductive "scale-based reasoning" and "data-driven reasoning". The features of our approach are demonstrated by discovering the basic formulae of the ideal gas law and Black's specific heat law from a set of numeric data. This approach may provide a basis to discover qualitative laws of ambiguous domains such as biology, psychology, economics and social science.*

Keywords: Scientific Discovery, First Principle Law, Scale-Based Reasoning, Data-Driven Reasoning, Measurement Theory.

1 Introduction

One of the early work to automatically discover formulae of physical first principles is a method called dimensional analysis that was based on **Product Theorem** [2], [1].

Product Theorem *Assuming absolute significance of relative magnitudes of physical quantities, the function f relating a secondary quantity to the appropriate primary quantities, $x, y, ...$ has the form: $f = Cx^a y^b z^c ....$, where $C, a, b, c, ...$ are constants.*

There is another important theorem that is called **Buckingham Π-theorem** [3], [1].

Buckingham Π-theorem *If $\phi(x, y, ...) = 0$ is a complete equation, then the solution can be written in the form $F(\Pi_1, \Pi_2, ..., \Pi_{n-r}) = 0$, where n is the number of arguments of ϕ, and r is the basic number of dimensions in $x, y, z.....$ For all i, Π_i is a dimensionless number.*

Basic dimensions are such dimensions as length $[L]$, mass $[M]$ and time $[T]$, scaling quantities independently of other dimensions in the given ϕ. This theorem can be used together with **Product Theorem** to obtain the oscillation period $t[T]$ of a simple pendulum from its stick length $l[L]$, gravity acceleration $g[LT^{-2}]$ and deviation angle θ [no dimension] (see Fig.1.). We can find two dimensionless quantities $\Pi_1 = t(g/l)^{1/2}$ and $\Pi_2 = \theta$, and derive the basic formula of the solution as $F(\Pi_1, \Pi_2) = F(t(g/l)^{1/2}, \theta) = 0$ based on the theorem. Using these dimensional analysis techniques, Bhaskar and Nigam introduced a concept "*regime*" which is a formula $\rho_i(\Pi_i, x, y, ...) = 0$ defining a dimensionless quantity Π_i[1]. In the above example, $t(g/l)^{1/2}$ and θ are the regimes. Further, they defined an "*ensemble*" which is a set of regimes contained in a complete equation $F(\Pi_1, \Pi_2, ..., \Pi_{n-r}) = 0$. In the current example, $F(t(g/l)^{1/2}, \theta) = 0$ is the ensemble. A regime refers to a decomposable subprocess. An ensemble stands for a complete physical process in the system. The dimensional analysis utilizes the physical insights into the objective system that is described by the unit dimension of each quantity. Another method to automatically derive physical formulae is symmetry-based approach which was proposed by Ishida[5]. He ap-

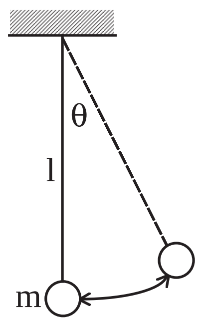

Figure 1: A simple pendulum

plied the principle of symmetry to physical domains. The system he developed heuristically searches for the invariant physical formula under a given set of isomorphic mappings. In the example of the simple pendulum, we can apply further constrains of symmetry on the form $F(t(g/l)^{1/2}, \theta) = 0$. One is phase translatory symmetry on t, and this gives $F(t(g/l)^{1/2}, \theta) = F((t(g/l)^{1/2} + 2m\pi, \theta)$, where m is an integer. Another is mirror symmetry of the time t and angle θ giving $F(t(g/l)^{1/2}, \theta) = F(-t(g/l)^{1/2}, -\theta)$. A formula satisfying these constraints is $\theta = \sin(t(g/l)^{1/2})$. As is evident, this method also has to utilize the explicit knowledge of physical characteristics of the object in terms of symmetry.

In contrast with these methods that are grounded on physical knowledge, a challenge has been made by Langley and Zytkow to discover the formulae of the first principles that govern the objective system [7]. They used a data-driven approach and developed BACON that discovers formulae by using heuristic search algorithm. The objects in various domains can be modeled because it does not use any a priori knowledge of the objects. However, the heuristics in the search algorithm have no firm theoretical bases, and the search is limited to enumerating only polynomial and meromorphic formulae. Accordingly, the set of the solutions obtained is not ensured to be sound and complete.

All the previous approaches employ the following assumption.

Assumption 1 *The relation among quantities under consideration is represented by a complete equation.*

Though Bhaskar and Nigam demonstrated the applicability of their dimension-based method to the systems consisting of multiple complete equations, the specification of a set of quantities is required for each complete equation in the framework, and thus this assumption must be maintained[1]. Their dimension-based approach also requires the following assumptions.

Assumption 2 *The type of scales of physical quantities is limited to ratio scale.*

Assumption 3 *Given a regime $\rho_i(\Pi_i, x, y, ...) = 0$, either one of the following conditions holds.*

i) It is a unique regime of a complete equation.

ii) For each quantity x in ρ_i, any other regimes do not contain x, or any other regimes are related in such a way that x does not change Π_i from outside of ρ_i.

Assumption 2 is the restatement of the assumption in **Product Theorem**, *i.e.*, the absolute significance of relative magnitudes of physical quantities. Although the quantities of the ratio scale are quite common in various domains, there is another scale type of quantities called as "*interval scale*" which is also widely encountered as explained later. **Assumption 3** was recently pointed out by Kalagnanam and Henrion[6]. The data-driven approach of BACON assumes the following environment of data measurement.

Assumption 4 *The measurements on the relation in any subset of quantities in a complete equation can be made while holding the other variables constant under an experimental environment, and the measured data can be sequentially used to reason the formula relating the variables.*

The objective of this paper is to propose a new approach to automatically discover formulae of first principles. Our approach lies in between the deductive approaches as represented by dimension-based and symmetry-based reasoning and the empirical approaches as represented by BACON. The following theoretical aspects removing the limitations of **Assumptions 2** and **3** are newly introduced in this paper.

i) The sound relations among quantities of ratio and interval scales within a regime are characterized, and **Product Theorem** is extended to reflect the relations.

ii) The structure of dimension is characterized for both ratio and interval scale quantities, and **Buckingham Π-theorem** is extended for the structure.

iii) The condition that each regime contains a set of quantities that are mutually exclusive in an ensemble is characterized (*i.e.*, the condition that a set of regimes forms a partition of the quantities), and an algorithm to identify such regimes is proposed.

The other two assumptions remain the same in our approach at present. On these grounds, our approach can derive a sound set of solutions of the formulae for each regime similarly to the dimension-based approach while still maintaining the advantage of the data-driven approach like BACON, *i.e.*, it does not require a priori insights into the objective system but only data that can be obtained by measurements. Thus, it can be applied to various domains and is not limited to physics.

2 Basic Principle of Scale-Based Reasoning

Since after Helmholtz originated a research field of "*measurement theory*" [4], many literatures have been published on that topic in the 20th century. Stevens defined the measurement process as "*the assignment of numerals to object or events according to rules*"

[10]. He claimed that different kinds of scales and different kinds of measurement are leaded, if numerals can be assigned under different rules. Two of the scale categories he defined are reproduced in Table 1. The interval scale and the ratio scale are the majorities of quantities in physical, psychological, economical and sociological domains. Examples of the interval scale quantities are temperature in Celsius and Fahrenheit, energy, entropy, time (not time interval), and sound tone (proportional to the order of white keys of a piano). The zero point level of their scales are not absolute, and are changeable by human's definitions. Examples of the ratio scale quantities are physical mass, absolute temperature, pressure, time interval, frequency, and currency value. Each has an absolute zero point, and the ratio of two different values x_1/x_2 is invariant against their unit change. The scale is different from the dimension. The scale just represents the definition of the measurement rule. Another point we should clarify is that dimensionless quantities are the quantities of absolute scale having the group structure of $x' = x$, because any change of units is not defined.

Luce claimed that the basic formula of the functional relation between any two quantities can be determined by the scale features of these two quantities, if the quantities are not coupled through any dimensionless quantities[8]. Suppose x and y are both ratio scale quantities, and y is defined by x through a continuous functional relation $y = u(x)$. Suppose the form of $u(x)$ is logarithmic, *i.e.*, $y = \log x$. We can multiply a positive constant k to x, *i.e.*, a change of unit, without violating the group structure of the ratio scale quantity x shown in Table 1. However, this leads $u(kx) = \log k + \log x$, and this fact causes the shift of the origin of y by $\log k$, and violates the group structure of y which is the ratio scale quantity. Hence, the functional relation from x to y must not be logarithmic. As the admissible transformations of x and y in their group structures are $x' = kx$ and $y' = Ky$ respectively, the relation of $y = u(x)$ becomes as $y' = u(x') \leftrightarrow Ky = u(kx)$. The factor K of the changed unit of y may depend on k, but it shall not depend upon x, so we denote it by $K(k)$. Consequently, we obtain the following constraints on the continuous function $u(x)$.

$$u(kx) = K(k)u(x),$$

where $k > 0$ and $K(k) > 0$, as these are the factors of the changed units. The constraints for the different combinations of the scale types are summarized on the fourth column in Table 2 [8]. Luce derived each solution of $u(x)$ under the condition of $x \geq 0$ and $u(x) \geq 0$. We extended his theorems to cover the negative values of x and $u(x)$, and the result is summarized on the last column in Table2. Because of the space limitation, we omit the proof for the results. For the detail, see the reference[11].

The impossibility of the definition of a ratio scale from an interval scale in Table2 is because the ratio scale involves the information of an absolute origin, but the interval scale does not. Luce gave some examples of the equations in Table2 [8]. The quantities entering into Coulomb's law, Ohm's law and Newton's gravitation law are all ratio scales, and the formula of each law is a power function which follows the formula of Eq.1 in the table. We see examples of Eqs.2.1 and 2.2 for laws associated with energy and entropy. The total energy U of a body having a constant mass m and moving at velocity v is $U = mv^2/2+P$, where P is the potential energy. If the temperature of a perfect gas is constant, then the entropy E of the gas as a function of the pressure p is of the form $E = -R\log p + E'$, where R and E' are Boltzmann's constant and a reference value of entropy respectively. In psychophysics, Fechner's law states that the sound tone s of human sensing (proportional to the order of white keys of a piano) is proportional to the logarithm of the sound frequency f, *i.e.*, $s = \alpha \log f + \beta$, where s is an interval scale, and f is a ratio scale. As an example of Eq.4, there is the relation $x = vt + x_0$ for a particle moving at its constant velocity v, where x is the position at the present time t and x_0 is the initial position x.

Finally, the following important consequence should be indicated. The detail of its proof is provided in the letterature[11].

Theorem 1 *An absolute scale quantity can have functional relations of any continuous formulae with other absolute scale quantities.*

For example, the behavior solution of the simple pendulum of Fig. 1 is $\theta = \sin(t(g/l)^{1/2})$. The triangular function sin which does not belong to Table 2 can hold, because θ and $t(g/l)^{1/2}$ are dimensionless, *i.e.*, absolute scale.

3 Theory and Method to Derive Law Equations

3.1 Scale-Based Reasoning within a Regime

This subsection describes the theory and the method of scale-based reasoning which uses a priori knowledge of quantity scales (not the knowledge of physics) to derive the formula of ρ_i for a given regime. **Product Theorem** is extended to include interval scale quantities. The principle of the extension is a certain symmetry that the relations given in Table 2 must hold for each pair of quantities in a regime[11].

Theorem 2 *Given a set of quantities* $Q = \{x_1, x_2, ..., x_m\}$ *forming a regime where some quantities are interval scales and the others ratio scales, the relation* $f = 0$ *among* $x_1, x_2, ..., x_m$*, has either one of*

Table 1: Scale types

Scale	Basic Empirical Operations	Mathematical Group Structure
Interval	Determination of equality of intervals or differences	Generic linear group $x' = kx + c$
Ratio	Determination of equality of ratios	Similarity group $x' = kx$

Table 2: Constraints and their possible equations satisfying the scale characteristics

No.	Scale Types: Independent variable	Scale Types: Dependent (Defined) variable	Constraints	Possible Relations
1	ratio	ratio	$u(kx) = K(k)u(x)$	$u(x) = \alpha_*\|x\|^\beta$
2.1	ratio	interval	$u(kx) = K(k)u(x) + C(k)$	$u(x) = \alpha \log \|x\| + \beta_*$
2.2				$u(x) = \alpha_*\|x\|^\beta + \delta$
3	interval	ratio	$u(kx + c) = K(k, c)u(x)$	impossible
4	interval	interval	$u(kx + c) = K(k, c)u(x) + C(k, c)$	$u(x) = \alpha_*\|x\| + \beta$

1) $k > 0, K(k) > 0, K(k, c) > 0, *c$ and C can be any real numbers.
2) The notations α_*, β_* are α_+, β_+ for $x \geq 0$ and α_-, β_- for $x < 0$, respectively.

the two forms.

$$f(x_1, x_2, ..., x_m) = (\prod_{x_i \in R} |x_i|^{a_i})(\sum_{x_j \in I_1} b_{*j}|x_j| + c_{*1}) + \sum_{x_k \in I_2} b_k|x_k| + c_2 \quad (i)$$

$$f(x_1, x_2, ..., x_m) = \sum_{x_i \in R} a_i \log |x_i| + \sum_{x_j \in I} b_j|x_j| + c_* \quad (ii)$$

Here, R is a set of quantities of ratio scale in Q, and I is a set of all quantities of interval scale in Q. Also, I_1 and I_2 are any partition of I where $I_1 + I_2 = I$.

Theorem 3 *If $R = \phi$, i.e., $I = Q$, in* **Theorem 2** *then the relation $f = 0$ among $x_1, ..., x_m$ has the following form.*

$$f(x_1, x_2, ..., x_m) = \sum_{x_j \in I} b_j|x_j| + c_*$$

Because of the space limitation, the proofs of **Theorems 2** and 3 are omitted. For the detail, see the reference[11]. The admissible formulae represented in **Theorem 2** do not involve the mixed form of $\alpha \log |x_i| + \beta_*$ and $\alpha_*|x_j|^\beta + \delta (i \neq j)$.

Now, we consider to derive the candidates of formula $f = 0$ of a given regime ρ, where the set of quantities except dimensionless Π in ρ is $Q = \{x_1, ..., x_m\}$. The following algorithm based on **Product Theorem** and the above **Theorems 2** and **3** derives the candidates.

Algorithm 1

(Step 1) $Q = \{x_1, ..., x_m\}$, $S = \phi$. Let R be a set of all quantities of ratio scale in Q. Let I be a set of all quantities of interval scale in Q.

(Step 2) If $I = \phi$ {
Based on **Product Theorem**, push the following to S.
$f(x_1, x_2, ..., x_m) = \prod_{x_i \in R} |x_i|^{a_i} + c_* = 0.$ }
else if $R = \phi$ {
Push the relation of **Theorem 3** to S.}
else {
Enumerate candidate relations of (i) in **Theorem 2** for all binary partitions $\{I_1, I_2\}$ of I, and push those candidates to S. Push the relation of (ii) in **Theorem 2** to S.}

The candidates are rested in the list S. The result of S is sound, since the soundness is ensured by **Product Theorem**, **Theorems 2** and **3**. The complexity of this algorithm is low except the enumeration of all binary partitions $\{I_1, I_2\}$ of I, where the complexity is $O(2^{|I|})$. The exchange of I_1 and I_2 essentially gives an equivalent relation, as it is easily understood by the form of the original relation (i) of **Theorem 2**. Therefore, the complexity reduces to $O(2^{|I|-1})$. In any case, it is not very problematic, because the size of a regime is generally quite limited.

We implemented this algorithm by using a commercial formula-processing package MATLAB [9]. This algorithm have been tested by various physical laws. The following is an example of the ideal gas equation which forms a unique regime. A regime involving four quantities of pressure p, volume v, mass m and temperature t is given, thus $Q = \{p, v, m, t\}$. The quantities p, v and m are ratio scales, while only t is an interval scale unless it is absolute temperature. We assumed the positive sign of p, v and m in advance, hence the solutions for their negative values were omitted. The algorithm figured out the two candidate relations. The first one comes from (i) of **Theorem 2** :

$$0 = c_1 p^{a_1} v^{a_2} m^{a_3} + b_1 t + c_2,$$

and the second one comes from (ii) of **Theorem 2** :

$$0 = a_1 \log p + a_2 \log v + a_3 \log m + b_1 * t + c.$$

From these, the following candidates were obtained.

$$p^{a_1} v^{a_2} = m^{-a_3} \left(-\frac{b_1 t + c_2}{c_1}\right).$$

$$p^{a_1} v^{a_2} = m^{-a_3} \exp(-b_1 t - c).$$

The former solution reflects the right formula of the ideal gas equation, when the temperature is not absolute one. Once the candidate formulae of a regime are determined, the correct formula and the values of its coefficients must be specified in data-driven manner.

3.2 Data-Driven Reasoning on Ensemble

Before proposing the data-driven reasoning on an ensemble, the definition of dimension, regime, ensemble and the consequence of **Buckingham Π-theorem** need to be re-examined. Within the conventional view, a basic dimension, D, of a quantity is defined by a basic unit, U, of the quantity, i.e., the basic dimension is represented as D(U). The value of a measured quantity is represented by the number of units equivalent to the amount of the quantity. For example, if the mass of an object is equal to the mass of seven basic units where each mass unit is named as $1kg$, then the mass of the object is said to be $7kg$. When we use another basic unit such as $1g$, then the measured value of the same object will be 1000 times larger. This definition is valid only for basic quantities of ratio scale. Basic quantities of interval scale has a bit more complex structure of dimensions. A basic unit and a *basic origin* are required to determine the value of temperature in Celsius. These unit and origin are different for temperature in Fahrenheit. Consequently, we need to extend the notion of a basic dimension as D(U, O) where O stands for a basic origin. In case of a basic quantity of ratio scale, O is constrained to be 0, while O can take an arbitrarily value for a basic quantity of interval scale.

Based on the above discussion, the notion of the structure of a general dimension consisting of multiple basic dimensions is also extended. For example, let us consider the total energy of a particle. The particle having a certain temperature is moving at a certain height in a certain velocity. Thus, its total energy E_t is:

$$E_t = E_h + E_p + E_m,$$

where E_h, E_p and E_m are contained heat energy, potential energy and kinematic energy respectively. Every energy has an identical unit of $[M][L]^2[T]^{-2}$ where $[M], [L]$ and $[T]$ are basic units of mass, length and time. On the other hand, E_h, E_p and E_m are interval scale, since E_h is defined by temperature measured on a reference temperature point $[T_o]$, E_p by a reference height level $[H_o]$ and E_m by the kinematic energy of a reference coordinate $[E_o]$. Every energy component has its own reference point, i.e. the basic origin. Because E_t is the summation of E_h, E_p and E_m, the dependency of the value of E_t to these basic origins has a linear form of $mc[T_o] + mg[H_o] + [E_o]$ where m is the mass of this particle, c the specific heat coefficient and g the gravitational acceleration. Accordingly, the structure of the dimension of E_t is represented as $D([M][L]^2[T]^{-2}, mc[T_o] + mg[H_o] + [E_o])$. The structure of a general dimension can be represented as $D(U_1^{\alpha_1} U_2^{\alpha_2} \cdots, \beta_1 O_1 + \beta_2 O_2 + \cdots)$ where $U_1, U_2, \cdots$ are basic units, and $O_1, O_2, \cdots$ are basic origins. This is because the relation among origins follows **Theorem 3** , while the relation among units follows **Product Theorem**.

This extended structure of the dimension requires to extend **Buckingham Π-theorem** as follows.

Theorem 4 (Extended Buckingham Π-theorem) *If $\phi(x, y, ...) = 0$ is a complete equation, then the solution can be written in the form $F(\Pi_1, \Pi_2, ..., \Pi_{n-r-s}) = 0$, where n is the number of arguments of ϕ, and r and s are the number of basic units and that of basic origins of the dimensions in $x, y, z.....$ For all i, Π_i is a dimensionless number.*

Proof.
For ease of notation, we assume that s basic origins are $O_1, O_2, ..., O_s$. If we shift the origins toward the negative directions by $\delta_1, \delta_2, ..., \delta_s$ respectively, the following primed measurements of x, y, ... are obtained based on the general structure of their dimensions.

$$\begin{array}{rcl} x' & = & x + \beta_1^x \delta_1 + \beta_2^x \delta_2 + \cdots + \beta_s^x \delta_s, \\ y' & = & y + \beta_1^y \delta_1 + \beta_2^y \delta_2 + \cdots + \beta_s^y \delta_s, \\ \cdots & \cdots & \cdots \end{array}$$

where βs are the factors to convert the shifts of origins *to the shifts on x's coordinate.*[1] *Since* $\phi(x, y, ...) = 0$ *is a complete equation, it must hold independent of the shift of the origins chosen to measure* $x, y, ...$[2]*; hence it follows that*

$$\phi(x', y', ...) = 0$$

or

$$\phi(x + \beta_1^x\delta_1 + \beta_2^x\delta_2 + \cdots + \beta_s^x\delta_s,$$
$$y + \beta_1^y\delta_1 + \beta_2^y\delta_2 + \cdots + \beta_s^y\delta_s, ...) = 0.$$

Differentiating this formula with respect to δ_1 *and setting all the* δ_i *to 0, we get:*

$$\beta_1^x\frac{\partial\phi}{\partial x} + \beta_1^y\frac{\partial\phi}{\partial y} + \cdots = 0$$

Now introduce new independent quantities:

$$x" = \frac{x}{\beta_1^x}, \qquad y" = \frac{y}{\beta_1^y}, \quad ...$$

In terms of these new quantities, the equation of partial derivatives can be rewritten as

$$\frac{\partial\phi}{\partial x"} + \frac{\partial\phi}{\partial y"} + \cdots = 0.$$

Let $\zeta"$ *be the last of the n quantities* $x", y", ...$ *Now introduce a set of quantities* z_i *such that:*

$$z_1 = x" - \zeta", \qquad z_2 = y" - \zeta", \quad ..., \quad z_n = 0.$$

Now we substitute the z_i *into the function* ϕ*. We then have:*

$$\phi(x", y", ..., \zeta") \equiv \phi(z_1 + \zeta", z_2 + \zeta", ..., \zeta").$$

It can be shown that function ϕ *is independent of* $\zeta"$*. Differentiating* ϕ *partially with respect to* $\zeta"$ *and using the above equation of partial derivatives, we can obtain* $\partial\phi/\partial\zeta" = 0$*. So,* ϕ *is a function of* $n-1$ *quantities z and we can write an equivalent function:*

$$\Psi(z_1, z_2, ..., z_{n-1}) = 0$$

Note that the arguments, z_i*, are dimensionless in the first basic origin. Now the process can be repeated for each remaining* $s-1$ *basic origins. Each time an origin is eliminated, the number of arguments in the function is reduced by 1. Thus when all s basic origins have been eliminated, we will be left with a function of the form:*

$$\Psi'(w_1, w_2, ..., w_{n-s}) = 0.$$

Each w_i *is dimensionless in terms of the basic origins, and so they have only basic units. By applying the conventional Buckingham* Π*-theorem to this complete equation, we obtain the final result.*

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

[1] For example, a shift of one unit temperature in Fahrenheit is 5/9 unit in Celsius.

[2] For example, an identical physical formula must hold for both units of Celsius and Fahrenheit.

This theorem ensures that we can remove the limitation of **Assumption 2**.

Another important subject is to overcome the limitation of **Assumption 3** that was pointed out by Kalagnanam and Henrion[6]. The process of identifying the formula of each regime $\rho_i(\Pi_i, x, y, ...) = 0$ is basically to find a relation among a subset of quantities in a complete equation while holding the condition that must hold outside of $\rho_i = 0$ constant as stated in **Assumption 4**. If **Assumption 3** does not hold, this operation is impossible because of the dependency among multiple regimes. This difficulty can be removed by introducing an idea of *pseudo-regime*.

Definition of pseudo-regime

A pseudo-regime is a subsystem, where the relation among quantities follows one of **Product Theorem**, **Theorem 2** and **3**, of a given complete equation.

Consider the example of convection heat transfer given by Kalagnanam et al. [6] The heat transfer from a fluid to a pipe wall takes place through convection when a fluid is forced through a pipe. A complete equation for this phenomenon under the turbulent flow is known as follows.

$$\Pi_1 = 0.023{\Pi_2}^{0.8}{\Pi_3}^{0.4},$$

where $\Pi_1 = \frac{hd}{k}, \Pi_2 = \frac{dv\rho}{\mu}$ and $\Pi_3 = \frac{c\mu}{k}$. Here, h is the convection heat transfer coefficient dependent to the other quantities, d and v are diameter of pipe and velocity of stream, and μ, ρ, c and k are the material quantities of the fluid, *i.e.*, viscosity, density, specific heat and thermal conductivity respectively. The number of quantities and that of the basic dimensions are $n = 7, r = 4$ and $s = 0$ respectively. Hence, three $(n - r - s = 3)$ regimes exist in this ensemble, and Π_1, Π_2 and Π_3 are called as Nusselt's, Reynold's and Prandtl's numbers in the thermal hydraulics domain. This example violates **Assumption 3**, because d, μ and k appear in multiple regimes. However, this equation is regarded as a unique pseudo-regime, because it can be rewritten to follow **Product Theorem** as:

$$\frac{k^{0.6}v^{0.8}\rho^{0.8}c^{0.4}}{hd^{0.2}\mu^{0.4}} - \frac{1}{0.023} = 0.$$

Accordingly, the data-driven search of a pseudo-regime can discover this formula without facing the difficulty pointed out by Kalagnanam and Henrion. In addition, these regimes can be decomposed into:

$$\Pi'_1 = d, \quad \Pi'_2 = k, \quad \Pi'_3 = \mu,$$

$$\Pi'_4 = \frac{h\Pi'_1}{\Pi'_2}, \quad \Pi'_5 = \frac{\Pi'_1 v\rho}{\Pi'_3} \quad \text{and} \quad \Pi'_6 = \frac{c\Pi'_3}{\Pi'_2}.$$

Because the set of quantities in each pseudo-regime does not have any intersection with the other pseudo-regimes, the data-driven discovery of these pseudo-regimes is also possible. The following theorem can be stated.

Theorem 5 *Given a complete equation* $\phi(x_1, x_2, ..., x_n) = 0$*, its decomposition into pseudo-regimes always exists where*

$$F(\Pi_1, \Pi_2, ..., \Pi_k) = 0 \quad and$$

$$\{\rho'_i(\Pi_i, x_{1_i}, x_{2_i}, ...x_{m_i}) = 0 | i = 1, ..., k\}.$$

Here $\{Q_i | Q_i = \{x_{1_i}, x_{2_i}, ...x_{m_i}\}, i = 1, ..., k\}$ *is a partition of entire quantity set* $Q = \{x_1, x_2, ...x_n\}$.
Proof.
If a regime of $\phi = 0$*, i.e.,* $\rho(\Pi, x_1, x_2, ...x_m) = 0$*, has a set of common arguments* S *with the other regimes, then the decomposition of the* $\rho = 0$ *into the following pseudo-regimes:*

$$\rho'_i(\Pi_i, x_i) = \Pi_i - x_i = 0 \quad for \quad x_i \in S$$

and

$$\rho'(\Pi, \{x_1, x_2, ...x_m\} - S) = 0$$

is always possible. By applying similar decomposition to the other regimes, every pseudo-regime becomes mutually independent. Hence at least, one decomposition of $\phi = 0$ *described in this theorem always exists.*

The quantity Π of a pseudo-regime may not be dimensionless, since a pseudo-regime does not have to consist of quantities that cancel out every dimensions. Therefore, the following assumption must hold.

Assumption 5 *The measurement for the data of the entire complete equation must follow a consistent unit system.*

Otherwise, the formulae of the ensemble may become invalid, since it is not invariant to the change of dimensions.

The algorithm to discover an ensemble and a set of pseudo-regimes involves a stage to identify pseudo-regimes, a stage to determine the arguments Πs of the ensemble and a stage to determine the formula of the ensemble. The following algorithm to discover the formula of a complete equation from the given data has been constructed.

Algorithm 2
(Step 1) $E = \{x_1, x_2, ...x_n\}$, $LE = \phi$ and $k = 1$.
(Step 2) Repeat until k becomes equal to n. {
  Repeat for every partition Γ_i of E where $|\Gamma_i| = k$. {
    Repeat for every $Q_{i_j} \in \Gamma_i (j = 1, ..., k)$. {
      Apply the algorithm 1 to Q_{i_j} to identify a pseudo-regime. Test each solution in S through the least square fitting to the measured data under some sets of values of quantities in $(E - Q_{i_j})$. If some solutions are accepted, substitute them to a list LQ_{i_j}.}
    If every $LQ_{i_j} \neq \phi$, let a list $L\Gamma_i = \{LQ_{i_j} | Q_{i_j} \in \Gamma_i, j = 1, ..., k\}$. Push $L\Gamma_i$ to LE.}
  If $LE \neq \phi$, go to (Step 3), else $k = k + 1$.}
(Step 3) Repeat for every $L\Gamma_i$ in LE. {
  Repeat for every LQ_{i_j} in $L\Gamma_i (j = 1, ..., k)$. {
    Repeat for every solution of a pseudo-regime, s_{i_j}, in LQ_{i_j}. {
      Determine an argument quantity $\Pi(s_{i_j})$ based on the coefficients of s_{i_j} evaluated through the least square fitting to the measured data.}}}
(Step 4) Repeat for every $L\Gamma_i$ in LE. {
  Take Cartesian products $LP_i = LQ_{i_1} \times LQ_{i_2} \times \cdots \times LQ_{i_k}$ in $L\Gamma_i$.
  Repeat for every $\{s_{i_1}, s_{i_2}, ..., s_{i_k}\} \in LP_i$. {
    Determine the formula $F(\Pi(s_{i_1}), \Pi(s_{i_2}), ..., \Pi(s_{i_k})) = 0$.}}

More concrete contents of this algorithm are demonstrated through an example of Black's specific heat law. This relates the initial temperatures of two substances T_1 and T_2 with their temperature T_f after they have been combined. This law has the formula of $T_f = (w_1 M_1/(w_1 M_1 + w_2 M_2))T_1 + (w_2 M_2/(w_1 M_1 + w_2 M_2))T_2$ where M_1 and M_2 are the masses of the two substances, and w_1 and w_2 are their specific heat coefficients. The conditions of $M_1 = 0.5 M_2$ and $w_1 = w_2$ are applied in our example. In (Step 1), the set of measured quantities E is set as $\{T_f, T_1, T_2, M_1, M_2\}$. (Step 2) is the process to enumerate all partitions of E where each subset of E is interpreted as a pseudo-regime. The goodness of the least square fitting of each candidate solution derived by the algorithm 1 is checked through the F-test which is a statistical hypothesis test to judge if the measured data follows the solution. If a parameter is close enough to an integer value, then the parameter is forced to be the integer, because the parameter having an integer value is quite common in various domains. Every partition Γ_i, where all of its subsets are judged to be pseudo-regimes, is searched in an ascending order of the cardinal number k of the partition. Once such partitions are found at the level of the certain cardinal number, (Step 2) is finished at that level to obtain the solutions of the ensembles involving the least number of pseudo-regimes. This criterion decreases the ambiguity of the formula of the ensemble by reducing the number of the absolute scale quantities in it. In the current example, only the partition of $\{\{T_f, T_1, T_2\}, \{M_1, M_2\}\}$ is accepted at the least cardinal number, $k = 2$. All quantities in the former pseudo-regime are of interval scale, and those in the latter are of ratio scale, and thus the formula of these pseudo-regimes are enumerated as:

$$T_f = b_1 T_1 + b_2 T_2 + c_1, \qquad M_1^{a_1} M_2^{a_2} + c_1 = 0.$$

Notice that the number of quantities n is 5 while $r = 2$ and $s = 1$ since temperature is interval scale and mass ratio scale. Therefore, the number of regime must be $n - r - s = 2$ according to the extended **Buckingham Π-theorem** which is consistent with the above result. Their more specific formulae are identified through the data fitting as follows.

$$T_f = b_1 T_1 + b_2 T_2, \qquad M_1 M_2^{-1} + c_1 = 0.$$

(Step 3) defines an argument Π for each pseudo-regime. The definition can be made in various ways. In our approach, a parameter in a pseudo-regime, which varies by the influence from the other pseudo-regimes, is chosen to be a Π, and the other variable parameters in the pseudo-regime are evaluated in terms of the Π. In the current example, both of b_1 and b_2 in the former pseudo-regime are observed to be variable depending on the values of M_1 and M_2. Accordingly, many data of $\{b_1, b_2\}$ are evaluated through fitting to the measured data of T_f, T_1 and T_2 under various values of M_1 and M_2. Then, b_1 is chosen to be the Π_1 of the pseudo-regime, and various formulae of $f(\Pi_1)$ are tested for b_2 through the F-test of the least square fitting to the data of $\{b_1, b_2\}$. The class of $f(\Pi_1)$ is limited to polynomial and meromorphic formulae in our current study. The following is the most simple formula accepted in the test.

$$b_1 = \Pi_1, \qquad b_2 = 1 - \Pi_1.$$

For the latter pseudo-regime, c_1 is uniquely chosen to be the Π_2. (Step 4) searches the relation of each ensemble found in the preceding steps. In the example under consideration, first, many data of $\{\Pi_1, \Pi_2\}$ are obtained by applying various combinations of values of $\{T_f, T_1, T_2, M_1, M_2\}$. Then various formulae of $F(\Pi_1, \Pi_2) = 0$ are tested for the ensemble while limiting the class of F to polynomial and meromorphic formulae. The most simple formula accepted is as follows.

$$\Pi_1 \Pi_2 - \Pi_1 - \Pi_2 = 0.$$

By combining above formulae, the familiar equation of the Black's specific heat law under the condition of $w_1 = w_2$ is obtained.

$$T_f = \frac{M_1}{M_1 + M_2} T_1 + \frac{M_2}{M_1 + M_2} T_2.$$

4 Conclusion

In this paper we have proposed a new method that enables us to automatically discover formulae of first principles. Our approach lies in between the deductive approaches and the empirical data-driven approaches. The major characteristics of our approach are summarized as follows.

i) The sound solutions of basic formulae of law equations within a regime are provided by using only the knowledge of quantity scales.

ii) An ensemble and its pseudo-regimes in the objective system are identified from the experimental data without any strong limitations.

iii) The applicability is not limited to well-defined domains because the method does not require a priori knowledge except the knowledge of quantity scales.

The scale-based reasoning may provide a basis to discover qualitative models of ambiguous domains such as biology, psychology, economics and social science.

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