Introduction to an Invariant Quantity Method①

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ABSTRACT

It is impossible, mathematically, to use a time series which is regarded as a set of observational facts of a dynamic system to reconstruct the particular system. Physically, however, with a few assumptions put, a dynamic system can be rebuilt approximately by means of observational facts. This is the goal of the so called invariant quantity method (IQM), whose research and experiment are of potential significance to atmospheric sciences.

Key words: Dynamic system and semiflow, Characteristic line of first order partial differential equation, Conservation law and invariant quantity

I. BACKGROUND AND PRINCIPLES

1. *Reasoning Sciences and Inverse Problem*

Mechanics and physics are examples of modern reasoning sciences and the reasoning is completed through analysis of a model that has been established. To make accurate reasoning, observation and experiment are no doubt an important approach. We may consider the problem another way, i.e., the mathematic model is unknown or determined partially, but the object of study is given only by observations. This leads to an inverse problem of research. Mathematically, inverse problems, e.g., algebraic or differential equations can be dealt with only when the category of a model has been understood, a condition that is still missing for some meteorological issues. The conception presented here is to treat them with practically no prerequisites available. This is the invariant quantity method, which may be just as well referred to as an inverse problem of experimentation or physical reasoning.

It is absolutely necessary to mention the basis whereon one such model is built. The usual form of a scientific model or a practical model is the representation of definite solutions. The establishment of a differential equation needs the consideration of the conservation law and infinitesimal analysis of the study object. The concept of physical conservation law can be greatly expanded in terms of general principles and techniques, which is indicated by the evolution of Newtonian mechanics into classical mechanics and sets up for physical study an extremely extensive mathematic framework, including the establishment of such branches as statistical mechanics and random differential equations.

Up to this point, use of conservation laws has been beyond the scope of mass, momentum or energy conservation. It is conceivable to discover more conservation laws from mathematic models. These laws will be important properties of a given object of study. To the contrary, some essential bases will be provided for the establishment of a particular model if several conservation laws of the object are definitely known.

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Put in a visual way, a reasonable mathematic model or a theoretical model for an object is identical to a group of principal conservation laws. In a sense, therefore, one of the goals of scientific reasoning or model research is to discover such laws. Obviously, the model establishment has no option but to seek the related conservation laws.

A conservation law generally refers to a time invariant differential equation with the evaluation of its solution unvaried as a function of time. The solution is also called an invariant quantity, the example being the sum of potential and kinetic energy of a freely falling body in a gravitational field.

2. *Invariant Quantities of a Differential Equation*

A first order linear partial differential equation has its solution over a curved surface consisting of a family of specified curves referred to as characteristic curves of the equation that serve as a general solution of a system of ordinary differential equations, called the characteristic equations of a partial differential equation that, in turn, has a simplest relation to the characteristic equations, thus leading to the fact that mathematically the solution to a first order partial differential equation is reduced to that of its related characteristic equations.

The invariant quantity method (IQM) is based on the inverse utilization of the relation. Here, we have to ignore some mathematic details and trouble in order to illustrate the IQM formally.

Let the following definite solution problem have solutions $u(t)$ and $v(t)$, viz.,

$$\begin{cases} \dot{u} = P(u,v,t) \\ \dot{v} = Q(u,v,t) \qquad t > 0 \\ u(0) = u_0 \quad v(0) = v_0, \end{cases} \tag{1}$$

which is also termed the governing equation of functions $u(t)$ and $v(t)$. Function $F(u,v,t)$ is trivial in such a way that $F=$const. is always available for all evaluations (u,v,t) of an independent variable.

Nontrivial function $A(u,v,t)$ exists for (1) but for the solution of (1) we find

$$A(u(t),\ v(t),t) = \text{const.} \tag{2}$$

so that function A is referred to as an invariant quantity of (1). Evidently, (1) may have multiple such quantities because we have from (2)

$$\frac{dA}{dt} = \frac{\partial A}{\partial u}\dot{u} + \frac{\partial A}{\partial v}\dot{v} + \frac{\partial A}{\partial t} = 0, \tag{3}$$

that is,

$$\frac{\partial A}{\partial u}P + \frac{\partial A}{\partial v}Q + \frac{\partial A}{\partial t} = 0. \tag{4}$$

Now, the invariant quantity of (1) is none other than a nontrivial solution to (4). Here, assume that a solution to (2) is always existent and we find more than one such quantity in (1).

Set two invariant quantities $A(u,v,t)$ and $B(u,v,t)$ to have been discovered from (1). By their functional independence at some point we mean in the neighborhood of the point (u_0, v_0, t_0)

$$\det\ S(A,B) = \begin{bmatrix} \frac{\partial A}{\partial u} & \frac{\partial A}{\partial v} \\ \frac{\partial B}{\partial u} & \frac{\partial B}{\partial v} \end{bmatrix} \neq 0.$$

Now, $u(t_1) = u_1$ and $v(t_1) = v_1$ can be approximately calculated. Invariant quantities A and B are both the solutions to (3), namely,

$$\begin{cases} \frac{\partial A}{\partial u}\dot{u} + \frac{\partial A}{\partial v}\dot{v} + \frac{\partial A}{\partial t} = 0, \\ \frac{\partial B}{\partial u}\dot{u} + \frac{\partial B}{\partial v}\dot{v} + \frac{\partial B}{\partial t} = 0, \end{cases} \tag{5}$$

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} = -S^{-1}\frac{\partial}{\partial t}\begin{bmatrix} A \\ B \end{bmatrix}, \tag{6}$$

$$S(A,B) = \begin{bmatrix} \frac{\partial A}{\partial u} & \frac{\partial A}{\partial v} \\ \frac{\partial B}{\partial u} & \frac{\partial B}{\partial v} \end{bmatrix}. \tag{7}$$

When A and B as functions of u, v, t are specified, A, B and $S(A,B)$ are the function or functional matrix of (u, v, t), and evaluated at (u_i, v_i, t_i) that are designated as A_i, B_i, S_i, respectively.

Let's deal with approximate calculation. Set $t_i = i, \Delta t_i = 1, \Delta u_i = u_{i+1} - u_i$ and $\Delta v_i = v_{i+1} - v_i$, we have

$$\begin{bmatrix} \dot{u} \\ \dot{v} \end{bmatrix} \rightarrow \begin{bmatrix} \Delta u_i \\ \Delta v_i \end{bmatrix} = \begin{bmatrix} u \\ v \end{bmatrix}_{i+1} - \begin{bmatrix} u \\ v \end{bmatrix}_i .$$

Therefrom the evolution equation (8)

$$\begin{bmatrix} u \\ v \end{bmatrix}_{i+1} = \begin{bmatrix} u \\ v \end{bmatrix}_i = S_i^{-1}\frac{\partial}{\partial t}\begin{bmatrix} A \\ B \end{bmatrix}_i \tag{8}$$

results and is called an evolution matrix with respect to (7).

With the aid of (8), we complete the calculation of

$$(u_0, v_0) \rightarrow (u_1, v_1) \rightarrow \cdots$$

Note in particular that the existence of S_i^{-1} is necessary for the evolution equation (8), which is equivalent to the nondegenerate matrix S_i, or in other words, A and B are functionally independent at $t = i$.

Then, evolution equation (8) does not present a linear extrapolation relation for the evolution matrix varying as a function of t so that S_i can be assumed to be an element of an evolution semigroup of an evolution equation.

It is easy for (8) to guarantee the independence of functions A and B, which will be dealt with later.

3. *Invariant Quantities*

In this part the importance of the IQM is illustrated.

Set $u(t) = e^t$, $v(t) = t^2 + t + 1$ and from $t = +\ln u (u > 0)$ it follows that

$$A(u,v,t) = t^2 + \ln u - v = 1,$$
$$B(u,v,t) = (\ln u)^2 + t - v = 1,$$

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$$S(A,B) = \begin{bmatrix} \frac{1}{u} & -1 \\ \frac{2}{u}\ln u & -1 \end{bmatrix},$$

$$\det S(A,B) = \frac{1}{u}(2\ln u - 1) \neq 0 \quad (u \neq \sqrt{e}).$$

The following properties are of note.

(1) Curve $L(u(t), v(t), t)$ is involved simultaneously in the curved surfaces $A=1$ and $B=1$ with the result that L is the intersecting line and determined in an approximate fashion from (8); (8) fails to work when two such surfaces are just tangential to each other, leading to the dependence of functions A and B at this point, (8) would yield poor results if the surfaces were so in an approximate manner. However, these situations are easily improved and as a problem will be treated below.

(2) The IQMs built upon $u(t)$ and $v(t)$ are many only with the reversibility of t in its neighborhood, viz., $u(t)$ (> 0) is reversible in this case. Specifically, invariant quantities of u and v have meaning only on a local basis. As will be shown later, the IQM allows to change at will in such quantities. Consequently, their localism will not prevent (8) from its use.

(3) For the nontrivial smooth function $F(x)$ or $G(x,y)$, $F(A)$ or $G(A,B)$ is still the invariant quantities of u and v. Nevertheless, A and $A(F)$ must be functionally dependent; so must A, B and $G(A,B)$; A and G or B and G are likely to be functionally independent.

Therefrom we come to the following inference.

$u(t)$ and $v(t)$ are functionally independent at t_0, wherefrom come a series of invariant quantities

$$A,B,C,D,E,\ \cdots$$

of which a set of any three functions are bound to be functionally dependent. For any such quantity, e. g., A, another one, say, B must be available, both being functionally independent at t_0. Probably, A and B are functionally dependent at t_1 but we can proceed to take another function, say, F to make A and E independent at t_1.

Property (1) describes the IQM's geometrical significance. Properties (2) and (3) can be proved by means of the implicit function theorem in the context of mathematic analysis.

4. *Invariant Nature of Evolution Equation*

The basis for making possible the IQM is provided by (2), (3) and the invariant nature of the evolution equation to be proven in this section.

Assume u and v to have pairs of invariant quantities A, B and C, D, and it can be formally proved that the evolution equation from $A-B$ pair is equivalent to that from $C-D$ pair.

Proof: A and B are functionally independent and from (3) we know the dependence of A, B and C so that $C=F(A,B)$ exists at t_0 and by analogy we get $D=G(a,b)$, wherein F and G are smooth functions. Note that the proof is not strict but acceptable in practice.

At first we compute the derivatives of functions C and D

$$\frac{\partial C}{\partial u}=\frac{\partial F}{\partial A}\frac{\partial A}{\partial u}+\frac{\partial F}{\partial B}\frac{\partial B}{\partial u}\ ,$$
$$\frac{\partial C}{\partial v}=\frac{\partial F}{\partial A}\frac{\partial A}{\partial v}+\frac{\partial F}{\partial B}\frac{\partial B}{\partial v}\ .$$

Then we deal with the derivative of D

$$S(C,D)=\begin{bmatrix}\frac{\partial C}{\partial u} & \frac{\partial C}{\partial v}\\ \frac{\partial D}{\partial u} & \frac{\partial D}{\partial v}\end{bmatrix}=\begin{bmatrix}\frac{\partial F}{\partial A} & \frac{\partial F}{\partial B}\\ \frac{\partial G}{\partial A} & \frac{\partial G}{\partial B}\end{bmatrix}\begin{bmatrix}\frac{\partial A}{\partial u} & \frac{\partial A}{\partial v}\\ \frac{\partial B}{\partial u} & \frac{\partial B}{\partial v}\end{bmatrix}$$
$$=\bar{S}(F,G)S(A,B).$$

Now we calculate the derivative with respect to t

$$\frac{\partial C}{\partial t}=\frac{\partial F}{\partial A}\frac{\partial A}{\partial t}+\frac{\partial F}{\partial B}\frac{\partial B}{\partial t}\ ,$$

$$\frac{\partial D}{\partial t}=\frac{\partial G}{\partial A}\frac{\partial A}{\partial t}+\frac{\partial G}{\partial B}\frac{\partial B}{\partial t} ,$$

$$\frac{\partial}{\partial t}\begin{bmatrix} C \\ D \end{bmatrix}=\bar{S}(F,G)\frac{\partial}{\partial t}\begin{bmatrix} A \\ B \end{bmatrix} ,$$

where matrix $\bar{S}$ is the Jacobi square matrix of F, G in relation to A, B.

To verify the equivalent evolution equations from the two sets of invariant quantities, the form of (5) is used to yield such equations (equivalent to (8))

$$S(A,B)=\begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix}+\frac{\partial}{\partial t}\begin{bmatrix} A \\ B \end{bmatrix}=0 , \quad (9)$$

$$S(C,D)=\begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix}+\frac{\partial}{\partial t}\begin{bmatrix} C \\ D \end{bmatrix}=0 . \quad (10)$$

The above expressions for derivatives are used to reduce (10) to the form

$$\bar{S}(F,G)S(A,B)\begin{bmatrix} \Delta u \\ \Delta v \end{bmatrix}+\bar{S}(F,G)\frac{\partial}{\partial t}\begin{bmatrix} A \\ B \end{bmatrix}=0 .$$

If $S(F,G)$ is nondegenerate, S of the above expression can be eliminated so that (10) is equivalent to (9). Finally, it is extremely easy to prove that, if A, B are independent, then the sufficient and necessary conditions for the independence of invariant quantities C, D are nondegenerate $\bar{S}(F,G)$ *insomuch as the evolution equation established from* C, D *is no doubt* independent, i.e., S must be nondegenerate. The above has formally illustrated the variant nature of the evolution equation.

The invariant nature lies in that theoretically, change of the invariant will not affect extrapolation result at all in terms of (8). But difference in calculation is allowed. Hence, we should choose the invariants in such a way that the number of conditions to yield the square matrix $S(A,B)$ is made smallest possible.

5. *Invariant Quantities of Whole Domain and Its Part with Basic Assumption*

Function $u(t)$ and $v(t)$ are defined over domain $(0,T)$, in which invariant $A(u,v,t)$ must be that over its subdomain (t_1, t_2).

If $u(t)$, $v(t)$ and $A(u(t),v(t),t)$ were analytical functions, then the invariant quantities over (t_1, t_2) would undoubtedly be those over $(0,T)$.

The IQM is designed just for the following problem:

(1) for $u(t)$ and $v(t)$, only their evaluations are known at a limited number of points, i. e.,

$$u(i)=U_i \qquad t=i=1,2,\cdots,n$$
$$v(i)=V_i$$

meaning that two sequences u_i and v_i of length n are known.

(2) functions u and v are the solutions of unknown governing equation (1), which is, however, unknown.

We have to deal with u_i, $v_i\,(i>n)$ or $u(t)$, $v(t)(n<t<T)$ under these conditions.

If, in fact, u and v have invariant $M(u,v,t)$ over $(0,T)$, then naturally in point set $(1,2,\cdots,n)$ inside $(0,T)$ it is invariant, too,

$$M(u_i, v_i, i)=\text{const.} \qquad i=1,2,\cdots,n$$

If not, the invariant is constant over $(1,2,\cdots,n)$, viz.,

$$A(u_i, v_i, i)=\text{const.}$$

which will no longer guarantee invariant A to be constant outside $(1,2,\cdots,n)$, a contradiction that exists in the IQM.

Basic assumption. Set the series (u_i) and (v_i), $i=1,2,\cdots,n$ to have invariant

$$A(u_i, v_i, i) = \text{const.}$$

and we will assume A to be the constant of $u(t)$ and $v(t)$ at $t>0$.

This assumption is acceptable in the sense that (u_i) and (v_i) are long enough to fully reveal the evolution information of $u(t)$ and $v(t)$. As for timestep $\Delta t=1$, it should be regarded as indicating the gradual change in the subject on its corresponding time scale. The proposed assumption is necessary and reasonable.

Up to this point, the principle behind the IQM has been fully introduced.

II. INVARIANT QUANTITIES OF SEQUENCES

Theoretically, from series (u_i) and (v_i) with length n can be constituted a countless number of pairs of independent invariants. For sufficiently large n, however, it is necessary to consider approximate invariants with a view to reduce computational cost though with the facilities available at present it is possible to acquire accurate invariants.

It would be a highly interesting subject to seek the algorithm for finding the invariants if the IQM is accepted. Given here is only a feasible scheme for getting them. As for the algorithm, it is not difficult to work out so that only the principle will be presented without details to be introduced.

1. *Accompanying Sequence*

Nontrivial function $f(x,y,z)$ is selected. (Note that hereafter t will be used as a subscript in place of i.) Let

$$w_t = f(u_t, v_t, t), \quad \text{with} \quad t = 1,2,\cdots,n$$

Sequence w_t is the accompanying series of (u_t) and (v_t) and f is called an accompanying function.

If, for example, we take $f(u,v,t) \equiv u$ or $g(u,v,t) \equiv v$, then (u_t) and (v_t) are the special case of the accompanying sequence and will be put together with the latter in the following discussion.

2. *Construction of Invariants*

(w_t) can be viewed as an n–dimensional vector. It is known that $(n+1)$ n dimensional vectors will be linearly dependent, leading to the idea of determining $(n+1)$ associated functions f_k, with $k=1,2,\cdots$, $(n+1)$ so that as many accompanying functions will result. Consequently, we have

$$(w_t^1), (w_t^2), \cdots, (w_t^{n+1})$$

At least a set of constants b_k will yield an invariant.

Thus we get

$$A(u,v,t) = \sum_{k=1}^{n+1} b_k (w_t^k) = \sum_{k=1}^{n+1} b_k f_k (u_t, v_t, t) = 0.$$

3. *Approximate Invariants and a Potential Problem*

If given series (u_i) and (v_i) are excessively long, then to seek invariants becomes difficult. In that case, approximate invariants should be taken into account.

The procedure is to project (u_i) and (v_i) of n dimensional vector into n–dimensional space $(N<n)$, so that

$$(u_i)\to(a_j),\ (v_i)\to(b_j)\qquad \begin{array}{l} i=1,2,\cdots,n \\ j=1,2,\cdots,n \end{array}$$

At this time it is enough to generate $(n+1)$ a ssociated functions from (u_i) and (v_i).

To realize the projection from n dimension to N dimension (or rather, linear mapping) is made possible through limited Fourier transform of (u_i) and (v_i) with the representations truncated to N terms. But this is not the only way. It is believed that a problem of much interest is involved.

Linear mapping in limited dimensional space lies in selecting a set of bases (vectors). The base of limited Fourier transform is only one of the selectable orthogonal bases.

Suppose that we have some intuitive knowledge of (u_i) and (v_i) e.g., a frequent "wave pattern", periodic or aperiodic, which is taken as the base, of which the research is of highly potential significance.

The procedure is presented below for seeking approximate invariants by means of limited Fourier transform.

Through limited Fourier transform of (w_t^k) with the representation truncated to N terms $(N<n)$ we have the approximation

$$(w_t^k)=f_k(u_t,v_t,t)=\sum_{j=0}^{N}a_j^k\Phi_j(t)$$

where $\Phi_0(t)\equiv1$, leading to merely $(N-1)$ basic functions Φ_j and N associated sequences $(w_t^1),(w_t^2),\cdots,(w_t^N)$, which are, separately expanded into N terms, eliminating Φ_j to get an approximate invariant

$$A(u,v,t)=\sum_{k=1}^{N}b_kf_k(u,v,t)=\text{const.}$$

III. APPLICATION OF IQM

The IQM's application is based on extrapolation or dynamic analysis of the series. To make formal agreement, all governing equations are reduced to autonomous forms, e.g.,

$$\begin{cases}\dot u=P(u,v)\\ u(0)=u_0\end{cases}.$$

Let $t=v(t)$, $\dot v=1$ and $v(0)=0$ with which the above are changed into

$$\begin{cases}\dot u=P(u,v)\\ \dot v=Q(u,v)=1\\ u(0)=u_0\qquad v(0)=0\end{cases}.$$

1. *First Order Equation*

Suppose that the governing equation is a system of first order autonomous equations, with P and Q unknown.

Limited measurement series (u_i) and (v_i) are known for u and v, respectively, and are in the form

$$\begin{cases}\dot u=P(u,v)\\ \dot v=Q(u,v)\end{cases}$$

From (u_i) and (v_i) is constructed an invariant A

$$\frac{\partial A}{\partial u}du+\frac{\partial A}{\partial v}dv=0,$$

from which the dependence of du and dv (or Δu and Δv) is given. With $v(t)$ known, $u_j\,(j>n)$ can be obtained through extrapolation.

2. *High Order Equation*

Suppose that a governing equation is in second order non autonomous form and P is unknown. Known is the limited series (u_i)

$$\ddot{u} = P(\dot{u},u,t)$$

Set $\dot{u} = v$ and $t = w$ and the series is changed to the following first order system

$$\begin{cases} \dot{u} = v \\ \dot{v} = P(u,v,t) \\ \dot{w} = 1 \ , \end{cases}$$

(u_i) is used to compute all components of (v_i), leading to (w_i) taking the form (1,2,3…), from which two invariants are found for extrapolating (u_i) and (v_i).

3. *Selection of Invariants*

Chosen from (u_i) and (v_i) are a group of invariants A^1, A^2, … , then, a group of the evolution matrix $S(A^k, A^l)\,(k \neq l)$ is formed by way of one–to–one pairs. To make the extrapolation $(u_i, v_i) \to (u_{i+1}, v_{i+1})$ possible, the number of conditions should first be calculated for the evolution matrix group, i.e., the number of condition for the matrix $S_i(A^k, A^l)$. (8) will be utilized for the extrapolation as a pair (A^k, A^l) is obtained that has the minimum number of the conditions.

IV. CONCLUDING REMARKS

1. The IQM is developed for analyzing measured series in a dynamic context, the extrapolation being one of the major goals.

2. If (u_i) and (v_i) are set to be the evaluations of the functions $u(t)$ and $v(t)$, respectively, at a limited sampling, then u and v are the definite solutions of the unknown governing equation.

3. The governing equation contains a countless number of invariant quantities.

4. The evolution matrix and equation are established on the invariants and it is then possible that the series extrapolation and dynamic dependence can be dealt with. The evolution equations for different invariants are equivalent to each other.

5. If the invariants of the series are those of $u(t)$ and $v(t)$ as well, then these quantities of the former can be found out in a precise manner but they are often the approximate invariants for practical purposes.

6. Construction of the IQM depends on the associated function, which is chosen at will.

7. Mathematically, the IQM is based on forming an evolution semigroup (matrix) for the problem of definite solutions to the governing equation. The IQM is responsible for nonlinear extrapolation.

The IQM is a portion of the multipart paper, the others to appear being Recurrent Similarity and Simple Form Representation that will provide a range of applications of the scheme presented in this article.

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