Theoretical and Empirical Construction of a Dynamical System

Wasaburo Unno
Research Institute for Science and Technology, Kinki University
Higashi-Osaka, Osaka 577 Japan

(Received Dec. 28, 1994)

Abstract

A set of simultaneous first-order ordinary differential equations with time is the standard formalism describing a dynamical system. Such standard formulation of a dynamical system can be derived in a straightforward way from the normal form of the general variational principle describing the conservation of mass, momentum, and energy. On the other hand, the principal component analysis can be employed to derive the standard form of a dynamical system empirically from the observed data set, if sufficiently large number of observational quantities are measured in sufficiently large number of times to construct multi-dimensional phase spaces both from the measured quantities and from their time derivatives. Examples are given for that are constructed the theoretical and the empirical derivations of the standard dynamical system formulation. Improved principal component analysis is emphasized for use in the global environment

Key words: Dynamical system; General variational principle; Principal Component Analysis

1 Introduction

The development of science is oriented mainly by the natural philosophy on one hand and by the natural history on the other hand. Study of a complex system, however, requires both approaches, since a complex system is difficult to be studied only by theoretical basis but also without guiding theoretical ideas. Modeling is indispensable for studying a complex system. In the theoretical approach, a model is introduced into the conservation equations for constructing a dynamical system. For this purpose, the modal expansion of variables introduced into the general variational formulation by Glansdorff and Prigogine (1964; 1965), will give a set of the amplitude equations forming a dynamical system. The turbulent convection will be studied in this way (Unno, 1968) as an example of a theoretical complex system. On the other hand, the modeling in a complex observational system should be made directly from the observational data, and this is achieved in principle by using the principal component analysis (Unno, 1989; 1991). Let us suppose that a sufficiently large number of well-defined principal components should completely represent a dynamical system. Then, if the time derivatives of these principal components are added to the extended principal component analysis, no new sensible principal components should appear. As the result, the time derivatives of the principal components are represented by the linear combination of the principal components. This is perhaps the way that we have taken unconsciously in performing studies in natural history. The use of the multi-dimensional phase space for embedding a dynamical system combined with the development of the computer technology seems to provide a systematic way to construct the natural history. The earth environment will be treated as an example of the complex observational system (Unno, 1993).

2 General Variational Principle

Conservation of mass, momentum, and energy is the first principle of the macroscopic physics. Glansdorff and Prigogine (1965) introduced the general variational principle to formulate the conservation law, using the evolutionary criterion that the entropy of the fluctuation around the average motion should increase towards the macroscopically realized motion. The entropy δS associated with the fluctuation of size δ is given by $(-W_{min}(\delta)/T)$. The minimum work, $W_{min}(\delta)$, is calculated by integrating, from 0 to δ with respect to Δ, the increase of the total energy caused by an increment Δ of a fluctuation of magnitude δ, $[\Delta(\delta\rho)$, $\Delta(\delta T)$ and $\Delta(\delta\mathbf{u})]$, of a mass element and by the associated change in the surrounding medium under a reversible thermodynamic change in which the total volume and the total momentum are conserved. The result is given by, (see Landau and Lifshitz, 1958),

$$W_{min}(\delta) = \frac{1}{2}[c_v T(\delta T/T)^2 + (\frac{\partial P}{\partial \rho})_T(\delta\rho/\rho)^2 + (\delta\mathbf{u})^2], \tag{1}$$

where c_v denotes the specific heat at constant density, and P, ρ, T and $\mathbf{u}$ are pressure, density, temperature and velocity, respectively. Since the probability of finding a fluctuation of magnitude δ is proportional to $\exp[\delta S/k]$, the subsequent evolution of a macroscopic state takes place in the direction of increasing the entropy,

$$d_t(W_{min}/T) \geq 0, \tag{2}$$

where the equality holds at the equilibrium. The evolutionary criterion for finding the equilibrium state is, therefore,

$$d_t W_{min} = 0, \tag{3}$$

higher orders in δ being neglected. Since the time scale of a fluctuation is normally much shorter than the time scale of the macroscopic evolution, Prigogine and Glansdorff (1964, 1965) considered that the equation (3) should hold also for general non-steady macroscopic evolution. Thus, the general variational principle is described by

$$\delta\Phi = \int dm[d_t W_{min}] = 0, \tag{4}$$

where dm denotes the mass element and

$$d_t W_{min}(\delta) = c_v(\delta T/T) d_t \delta T + (\partial_\rho P)_T(\delta\rho/\rho^2) d_t \delta\rho + \delta\mathbf{u} \cdot d_t(\delta\mathbf{u}). \tag{5}$$

Now, fluctuating quantities under the time derivatives can be replaced by the differences between the corresponding quantities with fluctuations and their ensemble averages without fluctuations. Since the time derivatives of the latter averages are governed by the macroscopic conservation equations, the time derivative of a fluctuating quantity turns out to be given by the formula which vanishes by the conservation law. For instance,

$$d_t \delta\rho = d_t \rho + \rho\nabla\cdot\mathbf{u}, \tag{6}$$

of which the right-hand side vanishes by the mass conservation. We finally obtain the general variation formula of hydrodynamics as follows,

$$\int dm[P_\rho \frac{P}{\rho}\frac{\delta\rho}{\rho^2}\{\frac{d\rho}{dt} + \rho\nabla\cdot\mathbf{u}\} + \delta\mathbf{u}\cdot\{\frac{d\mathbf{u}}{dt} + \frac{1}{\rho}\nabla P - \mathbf{F}\}$$

$$+ \frac{\delta T}{T}\{c_v\frac{dT}{dt} - \epsilon + \frac{1}{\rho}\nabla\cdot\mathbf{H} + P_T\frac{P}{\rho}\nabla\cdot\mathbf{u}\}] = 0, \tag{7}$$

where ϵ, $\mathbf{H}, \mathbf{F}$, P_T and P_ρ denote the nuclear energy generation, the thermal energy flux, the viscous force, $[d(\log P)/d(\log T)]_\rho$ and $[d(\log P)/d(\log\rho)]_T$, respectively. The conservation of mass, momentum, and thermal energy is obvious in the above integral which should vanish for arbitrary variations of $\delta\rho, \delta\mathbf{u}$ and δT.

An alternative expression of equation (4) to equation (7) is possible by using P and S as dynamical variables instead of ρ and T, as follows,

$$\int dm[\frac{\delta P}{\rho}\{\frac{1}{\Gamma_1 P}\frac{dP}{dt} + \nabla\cdot\mathbf{u} - \frac{\nabla_{ad}}{P}(\rho\epsilon - \nabla\cdot\mathbf{H})\}$$

$$+\delta\mathbf{u}\cdot\{\frac{d\mathbf{u}}{dt} + \frac{\nabla P}{\rho} - \mathbf{F}\} + \frac{\delta S}{c_P}\{T\frac{dS}{dt} - \epsilon + \frac{\nabla\mathbf{H}}{\rho}\}] = 0, \tag{8}$$

where $\Gamma_1 = (d\log P/d\log\rho)_S$, $\nabla_{ad} = (d\log T/d\log P)_S$ and S denotes the specific entropy, and c_P the specific heat at constant pressure. Another formula that is the simplest and more often used is the mixed representation, that is,

$$\int dm[\frac{\delta P}{\rho}\{\frac{1}{\rho}\frac{d\rho}{dt} + \nabla\cdot\mathbf{u}\} + \delta\mathbf{u}\cdot\{\frac{d\mathbf{u}}{dt} + \frac{\nabla H}{\rho} - \mathbf{F}\}$$

$$+\frac{\delta T}{T}\{T\frac{dS}{dt}-\epsilon+\frac{\nabla\cdot\mathbf{H}}{\rho}\}]=0. \quad (9)$$

The above three formulae are equivalent with each other. The last one which is the most convenient for many other purposes, however, is not appropriate for deriving the amplitude equations in the following way. The other $(P, S, \mathbf{u})$ or $(\rho, T, \mathbf{u})$ representation can better be used for the construction of the dynamical system, depending on the physical property of the system. For the turbulent convection phenomena such as the stochastic excitation of the solar 5-min oscillation and the Lorenz chaos in meteorology, the $(P, S, \mathbf{u})$ representation may well be employed, since the entropy perturbation is the key factor of these phenomena. We now turn to discuss the turbulent convection phenomena by means of the modal expansion technics.

3 Linear Modal Expansion

Construction of a set of amplitude equations is the standard formalism of a dynamical system, (see Buchler, 1993a,b; Spiegel, 1993). We express each dynamical variable as the sum of the equilibrium part and its Lagrangian variation so that

$$P=P_0+P_1,\quad S=S_0+S_1,\quad \text{and}\quad \mathbf{u}=\mathbf{u_0}+\mathbf{u_1}, \quad (10)$$

and decompose the Lagrange variation into linear eigen-modes as follows,

$$P_1=\sum_{i=1}^{n}P^{(i)},\quad S_1=\sum_{i=1}^{n}S^{(i)},\quad \text{and}\quad \mathbf{u_1}=\sum_{i=1}^{n}\mathbf{u}^{(\mathbf{i})}. \quad (11)$$

Variations can be either Eulerian or Lagrangian. We employ here Lagrangian for the sake of formal simplicity, although Eulerian is preferred for nonlocal phenomena like the convection. Mathematically, the authogonality of the eigen-modes and the completeness of the eigen-mode expansion (11)are not proven. In practice, however, the authogonality and completeness are understood as the modeling of a complex system.

We are now interested not in the equilibrium configuration but in the dynamical system formed by the Lagrange variations. We therefore take only those parts of the general variational equation (8) that are related to the Lagrange variations. We have

$$\int dm[\frac{\delta P^{(i)}}{\rho}\{\frac{1}{\Gamma_1 P}(d_t P^{(i)}-a_{Pj}Q_j^{(i)})+(NL)_P^{(i)}\}$$
$$+\delta\mathbf{u}^{(i)}\cdot\{(d_t\mathbf{u}^{(i)}-a_{\mathbf{u}j}Q_j^{(i)})-(NL)_{\mathbf{u}}{}^{(i)}\}$$
$$+\frac{\delta S^{(i)}}{c_P}\{T(d_t S^{(i)}-a_{Sj}Q_j^{(i)})-(NL)_S^{(i)}\}]=0, \quad (12)$$

where $Q_j^{(i)}=(P^{(i)},\ S^{(i)},\ \mathbf{u}^{(i)})$, and a_{kj} denotes the matrix element which involves the equilibrium values only, and $(NL)_Q^{(i)}$ the nonlinear terms belonging to the $Q^{(i)}$ equation. The explicit derivation of the matrix a_{kj} and the nonlinear terms is not given in the present study.

By solving the eigen-value problem for the linear stability analysis, we can transform the above variational equation into the following standard form,

$$\int dm\sum_{j=1}^{n}[\delta X_j^{(i)}\{d_t-n^{(i)})X_j^{(i)}+(NL)_j^{(i)}\}]=0, \quad (13)$$

where the i-th eigen-value of the matrix $((a_{kj}))$ is the growth rate (generally complex) denoted by $n^{(i)}$, and

$$X_1^{(i)}=P^{(i)}/(\Gamma_1 P\rho)^{1/2},\quad \mathbf{X}_2^{(i)}=\mathbf{u}^{(i)},$$
$$\text{and}\quad X_3^{(i)}=S^{(i)}/(c_P/T)^{1/2}. \quad (14)$$

4 Amplitude Equations

Any parameter included in the variable $X_j^{(i)}$ can be taken as a variational parameter, and the resulting equation from the general variation equation (13) will give an equation to determine that parameter. In particular, for obtaining the amplitude equation, the natural choice will be on the growth rate $n^{(i)}$ included in the $\exp(n^{(i)}t)$ factor in $X_j^{(i)}$. Omitting the common factor t in the integrand, we have finally,

$$d_t \int dm(X_j^{(i)})^2 = 2\int dm[n^{(i)}(X_j^{(i)})^2 + X_j^{(i)}(NL)_j^{(i)}], \quad (15)$$

$(i = 1, 2, ...; j = P, S, \mathbf{u})$.

In the case of the Lorenz chaos, only three variables corresponding roughly to the horizontal pressure gradient, vertical velocity, and the vertical entropy gradient are chosen to represent the system. The corresponding amplitude equations are, therefore, different from the above normal form. Linear transformation of variables decomposes the system in three linearly independent eigen-modes of which one mode is neutral and the other two are stable and unstable. Nonlinearity first affects the neutral mode forming the global structure of the attractor that is primarily characterized by the stable (attractor forming) and unstable (strangeness giving) modes. Nonlinear transformation to visualize the structure of nonlinear terms seems to be effective for further study of the nonlinear behavior (Spiegel, 1993).

The stochastic excitation of the solar 5-min oscillations is another problems to be studied as a complex dynamical system. There are thousands of oscillation modes possibly excited stochastically by the turbulent convection in or near the edge of the convection zone. These oscillations are of the nonradial p-modes, while the convection is basically of the unstable g-modes or the g_+ modes in origin. The difficulty of the problem lies in the fact that not only the statistical properties of turbulent motions but also the variations of the phase relations among individual turbulent elements are involved in the problem. The dynamical system approach with appropriate modeling of turbulent eddies should be taken (Buchler,1993b).

5 Multi-Dimensional Representation

Before entering into the dynamical system formalism for the empirical data, we have to define the multi-dimensional phase space as the working field of complex dynamics. Let us consider the global environment as an example of a complex system to be studied empirically. Pressure, temperature, humidity, solar energy flux, rain fall, wind speed, etc. are supposed to be monitored daily at various places on the earth. The first thing to do is to homogenize data for the systematic differences due to the observed position and daily and seasonal variations. This can be done empirically, using the average value and the standard deviation of the observed quantity for normalization. We assume here this has already been done. To study the global environment, annual averages of various data may be used. For one observed quantity, however, we can derive many annual averages such as for the quantity itself, its longitudinal and latitudinal gradients, and its Laplacian, and all of their daily and seasonal amplitudes of variations. If we have 6 quantities to observe and 12 annual averages for one observed quantity, we can construct the phase space of 72 dimensions. Therefore, if the dynamical system moves in the manifold of 35 dimensions or lower, the phase space thus constructed may well embed the manifold in sufficient detail, provided that the observations are made at some hundred places in some 10 years of time span. ((2D+1)-dimensional space is required for embedding a D-dimensional chaotic system, (Takens, 1981).) Let Q_k (k=1,2,..,n) denote those (e.g. 72) normalized annual average quantities with the weight of observation, w_k. The weight w_k may be taken to be $[1+(\text{uncertainty measure/probable error})^2]^{-1}$. Then, we can plot one point (or more exactly a probability density distribution corresponding to w_k) in the embedding phase space for each observing site for each year. However, for convenience of the principal component analysis (PCA), we map the phase space to the normalized one by means of the transformation:

$$q_k = [Q_k - < Q_k >]/\sigma_k, \quad (k = 1, 2, .., n), \quad (16)$$

where

$$< Q_k > = (1/\sum_{i=1}^{N} w_k) \sum_{i=1}^{N} w_k Q_k^{(i)}, \quad (17)$$

and

$$\sigma_k^2 = (1/\sum_{i=1}^{N} w_k) \sum_{i=1}^{N} w_k [Q_k^{(i)} - < Q_k >]^2, \quad (18)$$

$Q_k^{(i)}$ being the Q_k value at the i-th (site and year), (i=1,2,..,N).

6 Improved Principal Component Analysis

In the following section, we construct a set of dynamical system equations out of the PCA of empirical data. There are, however, two drawbacks in that formalism. One is that the resulting dynamical system equations are linear in q_k and, therefore, cannot take account of the nonlinear effect. However, if the functional forms of the nonlinear terms are known either theoretically or empirically, or by trial and error, we include the functional form as a new member in Q_k. Improvement of PCA in this direction is not discussed in the present paper. The second drawback, on the other hand, lies in the fact that so many data are uncertain or incomplete but are important as a whole to determine the behavior of the complex system, and either inclusion or omission of the poor data results in the poor determination of the principal components. Improved PCA (IPCA) has been proposed in Unno and Yuasa (1992) as sketched below.

We have a primary data set $(q_k^{(i)}, w_k^{(i)})$, (i=1,2,...,N). Now, we add artificial data as $(x_k^{(i)}, v_k^{(i)})$ with

$$v_k^{(i)} = 1 - w_k^{(i)}. \tag{19}$$

These virtual data should be determined simultaneously and consistently with the IPCA by the condition that the whole data set attains the maximum probability distribution under the following statistical constraints,

$$\sum_{i=1}^{N} v_k^{(i)} x_k^{(i)} = 0, \quad \text{and} \quad \sum_{i=1}^{N} v_k^{(i)} {x_k^{(i)}}^2 = \sum_{i=1}^{N} v_k^{(i)}. \tag{20}$$

The principal components are the axes of the ellipsoidal distribution of datum points, and are the eigen-vectors of the correlation matrix $((r_{jk}))$,

$$((r_{jk})) = \sum_{i=1}^{N} (w_j^{(i)} q_j^{(i)} + v_j^{(i)} x_j^{(i)})(w_k^{(i)} q_k^{(i)} + v_k^{(i)} x_k^{(i)}), \tag{21}$$

such that

$$p_l = \sum_{j=1}^{n} \mu_{lj}(w_j q_j + v_j x_j), \tag{22}$$

where the direction cosines μ_{lj} are given by the condition that the squared norm of the eigen-vector, $\sum_{i=1}^{N}[p_l^{(i)}]^2$, be extremum for the variation of μ_{lj} under the constraints that $\sum_{j=1}^{n} \mu_{lj}^2 = 1$. Note that

$$p_l^2 = \sum_{j=1}^{n} [\mu_{lj}^2 (w_j q_j^2 + v_j x_j^2)$$

$$+ 2 \sum_{k>j} \mu_{lj}\mu_{lk}(w_j q_j + v_j x_j)(w_k q_k + v_k x_k)]. \tag{23}$$

The variation function determining the eigen-vector $((\mu_{lj}))$ is given by

$$S = S_0 - (\lambda_l/2)[\sum_{j=1}^{n} \mu_{lj}^2 - 1], \tag{24}$$

where

$$S_0 = (1/2N)\sum_{i=1}^{N}[p_l^{(i)}]^2 = \sum_{j=1}^{n}[(1/2)\mu_{lj}^2 + \sum_{k<j} \mu_{lj}\mu_{lk} r_{jk} \tag{25}$$

The unknown direction cosines μ_{lj} are the variation parameters, and the eigenvalue λ_l is the Lagrange multiplier of the conditional variation. The resulting eigen-value equations are given by

$$\sum_{k=1}^{n}[(1-\lambda_l)\delta_{jk} + r_{jk}(1-\delta_{jk})]\mu_{lk} = 0, \quad (j = 1, 2, ..., n \tag{26}$$

Solving for λ_l, we also obtain $((\mu_{lj}))$ by the standard linear algebra.

Now, it is easy to show that the mean-square dispersion of p_l is equal to λ_l on account of the above eigen-value equations. The probability of finding a set of principal components $(p_1, p_2, ..., p_n)$ in a volume element $dp_1\ dp_2 ... dp_n$ obeys the ellipsoidal distribution

$$W(\mathbf{p})(dp)^n =$$

$$[(2\pi)^n \prod_{l=1}^{n} \lambda_l]^{-1/2} \exp[-\sum_{l=1}^{n}(p_l^2/2\lambda_l)](dp)^n. \tag{27}$$

The variation function for determining $x_j^{(i)}$ is, therefore, given by

$$W = \sum_{i=1}^{N} W^{(i)} = \sum_{i=1}^{N}[-(1/2)\sum_{l=1}^{n}(p_l^{(i)})^2/\lambda_l], \tag{28}$$

p_l^2 being given by equation (23). Taking the variation $\delta x_j^{(i)}$, we obtain

$$\delta W/\delta x_j^{(i)} =$$

$$-v_j^{(i)}\sum_{l=1}^{n}(1/\lambda_l)[\mu_{lj}^2 x_j^{(i)}+\sum_{k\neq j}\mu_{lj}\mu_{lk}(w_k^{(i)}q_k^{(i)}+v_k^{(i)}x_k^{(i)})] = 0, \quad (29)$$

$(j = 1, 2, ..., n)$. The solution of this set of simultaneous algebraic equations gives $x_j^{(i)}$ in linear combination of $q_k^{(i)}(k = 1, 2, .., n)$. Then, our improved data set will be $[w_k^{(i)}q_k^{(i)} + v_k^{(i)}x_k^{(i)}]$ (k=1,2,...,n; i=1,2,..,N) with the weight of $[1 + w_k^{(i)}]/2$. The IPCA will be performed with the improved data set.

7 Construction of a Dynamical System by PCA

In the above PCA, we have plotted N points in the n-dimensional phase space, assuming that n $\geq$ (2D+1), where D denotes the correlation dimension of the dynamical system under consideration. Now, we increase the dimension of the embedding space from n to 2n by adding the time derivative for each $Q_k^{(i)}$ to the primary data set. Then, repeating the same procedure as explained in the preceding sections, we obtain 2n principal components. Among these principal components, however, those components that have the significantly large (≥ 1) eigen-values should have already been obtained, since the embedding dimension n of the first PCA was sufficiently large. Identification of new significant principal components with the old ones should give the amplitude equations as follows,

$$(d_t q)_{k'} = \sum_{l=1}^{n}\mu_{lk'}^{(2)}p_l = \sum_{l=1}^{n}\sum_{j=1}^{n}\mu_{lk'}^{(2)}\mu_{lj}q_j, \quad (30)$$

where $(d_t q)_{k'}$ denotes the normalized time derivative of Q_k, and $\mu_{lk'}^{(2)}$ the direction cosine between the $(d_t q)_{k'}$ axis and the p_l vector in the second PCA. In the original units, the above equation is rewritten as

$$d_t(Q_k - < Q_k >) =$$

$$\sum_{l=1}^{n}\sum_{j=1}^{n}\mu_{lk'}^{(2)}\mu_{lj}(\sigma_{k'}/\sigma_j)(Q_j - < Q_j >), \quad (31)$$

where k'= n+k in the second PCA, and $\sigma_{k'}$ denotes the rms dispersion of $d_t Q_k$. The set of these equations (k=1,2,..,n) constitutes the required empirical construction of a complex dynamical system.

8 Conclusion

The set of the amplitude equations defining a dynamical system is formulated theoretically, using the general variational principle and the linear mode expansion for the purpose of modeling the system. The amplitude equations can be regarded as the copy of the stationality of the minimum work in the positive-definite normal form. This seems to be the reason why the general variational principle can be useful in studying the dynamical system. Also, it is shown in the present study that the dynamical system formalism can be obtained empirically, using the principal component analysis applied to various observational data and their time derivatives. These two formalisms should open the way to study complex dynamical systems in the natural philosophy and in the natural history. In this paper, emphasis has been put especially on the IPCA which could remedy the difficulty of incompleteness of data in treating diversity of nonsystematic observations in the global environment problem. Wider application of the method, however, would be expected in various fields of natural and social sciences.

References

[1] Buchler, J.-R., 1993a, in *Nonlinear Phenomena in Stellar Variability*, eds. M.Takeuti and J.-R.Buchler, 9.

[2] Buchler, J.-R., 1993b, *Astron.Astrophys.* **280**, 157.

[3] Spiegel, E.A., 1993, in *Nonlinear Phenomena in Stellar Variability*, eds. M.Takeuti and J.-R.Buchler, 33.

[4] Unno, W., 1968, *Publ.Astron.Soc.Japan* , **30**, 356.

[5] Unno, W., 1989, *Sci.Tech., Kinki Univ.*, No.1, 41.

[6] Unno, W., 1991, *Sci.Tech., Kinki Univ.*, No.3, 41.

[7] Unno, W. and Yuasa, M., 1992, *Astrophys. Space Sci.*, **189**, 271.