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Physical Langevin model and the time-series model in systems far from equilibrium

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To bridge the gap between a physical Langevin equation and a stochastic equation used in the time-series analysis, and to clarify the physical foundations of the latter, the time-series model from the Langevin equation is derived with the aid of two manipulations—elimination of irrelevant variables and projection of state variables upon a space spanned by observed quantities. The order of the two manipulations is shown to be important to find an equation called the Kalman filter in control theory. All the results are summarized in a concise schematic diagram which relates various models and equations established so far in different fields.

I. INTRODUCTION

We shall consider in the present paper macroscopic steady-state systems such as chemical plants, nuclear plants, and biological systems. They are open systems, and usually have complicated reaction networks. From the physical viewpoint[1-3] as well as in the engineering aspect,[4] such a macroscopic system may be described by a set of linear Markovian Langevin equations, if we know a sufficient number of state variables necessary for the Markovian description. In large systems mentioned above, however, some variables cannot be measurable and the dimension of multivariate data is restricted to ten or a hundred, even if modern digital computers are used for the analysis. Thus, the information contained in the system is contracted, and the basic equations for the observable state variables are then non-Markovian, because of the elimination of the unobservable or hidden state variables. The contraction of information in a macroscopic world is, therefore, an interesting topic as in the statistical physics[5,6] of a microscopic world. We shall consider a nuclear reactor as a concrete example of the above-mentioned engineering plants. It is known[7] that in a simple model the state of a subcritical nuclear reactor is described by Langevin equations for two macroscopic variables, total number of neutrons, and that of delayed-neutron precursors. The time evolution of neutrons can be detected by a compensated ionization chamber equipped in the reactor core, while that of precursors is not detected directly. Thus we have a discrepancy that the theory describes the system in terms of the two physical variables whereas the experiment observes it through only one variable. The discrepancy is serious since the hidden variable—the delayed neutron precursors—plays an important role in reactor control and safety. Therefore, it is necessary to know the temporal behavior of precursors by analyzing neutron signal. In other words, it is important to identify the system by processing information contained in observed data, in order to understand physical phenomena occurring in the system.

The time-series analysis[8] provides a useful method for this identification. In this analysis, a basic model is assumed to be linear and stationary. The system is identified with multivariate time-difference equations, such as an AR (autoregressive) model and an AR-MA (autoregressive moving average) model. The basic structure of the models is non-Markovian. Namely, the AR-MA model is

$$y(n)=\sum_{i=1}^{M} A_i y(n-i)+\eta(n)+\sum_{j=1}^{L} B_j \eta(n-j)\ , \tag{1}$$

where $y(n)$ is an observable state vector, matrices A_i express autoregressive effects, $\eta(n)$ is the residual with white noise, and the last term is the one with colored noise. The order M represents the non-Markovian effect. The order L expresses the nonwhiteness. If the noise force is white ($L=0$), an AR-MA model reduces to the AR model. The orders M and/or L are fixed by information criteria such as FPE (Ref. 9) (final prediction error) and AIC (Ref. 10) (Akaike's information criterion). Then, the coefficient matrices of the model are determined from correlation functions of observed time-series data.

The time-series model can provide us with several statistical properties of system, e.g., power spectral density, coherence function, impulse response function, and relative power contribution of noise forces. Successful applications have been reported in many fields. For example, in the case of a cement rotary kiln[11] the observable vector consists of cooler pressure, exit gas temperature, and kiln drive power; in the case of a nuclear power reactor[7] the variables are number of neutrons, vapor pressure, and coolant temperature. Control of such an engineering plant becomes easier by fitting a time-series model to data obtained from the system. The time-series model is applied also to the analysis of the rotation of the Earth to estimate[12] the power spectrum of the Chandler wobble. Furthermore, it is used to forecast concentration of air pollution by analyzing the atmosphere which is a large and open system.

On the other hand, time-series analysis has the disadvantage that the physical processes are not clarified at all because of its methodical nature. It treats a complicated actual system as black box; a time-series model is determined from observed data in the manner as in the method of least-squares analysis. Therefore, the physical understanding[13] of the model is needed for practical system identification and for making a reliable diagnosis possible.

Our interest in this paper is how an "empirical" equation like Eq. (1) is related to physical equations that describe the actual phenomena occurring in a system far from equilibrium. We have the following questions.

(a) Though there are many models used in the time-series analysis, which type of equation is the most reasonable for describing a system far from equilibrium from the viewpoint of statistical physics?

(b) Once a system is identified by a model, then the characteristics of the model should be related to the phenomena occurring in the system. How should the orders of the model be affected from elemental processes involved in the phenomena? How should the coefficients of the model be connected to transition probabilities associated with the phenomena?

(c) How should the noise force $\eta(n)$ in Eq. (1) be related to the physical noise force?

We, thus, hope to bridge the gap between a physical model and a time-series model by clarifying the physics involved in the time-series model. To derive a time-series model, we shall start with a physical Langevin equation, make a coarse graining in time, eliminate irrelevant variables, and project relevant variables on a space spanned by observed variables. It is also shown that, if the projection is made before eliminating the irrelevant variables (i.e., if the irrelevant variables are also projected), we obtain the same model via a Kalman filter well known in control theory. The manipulations and equations are summarized in the diagram of Fig. 1. This schematic diagram helps us understand the physical meaning of the time-series model. It should finally be mentioned that the present approach is useful not only for identification but also for diagnosis as in the noise analysis in nuclear reactors.[7,14]

In Sec. II, a multivariate AR-MA model will be derived from a Langevin equation. The relationship among the Langevin equation in physics, the AR-MA model in the time-series analysis, and the Kalman filter in control theory will be clarified in Sec. III.

II. PHYSICAL FOUNDATION OF AR-MA MODEL

A. Non-Markovian equation

In a macroscopic world, van Kampen[1] and Kubo *et al.*[2] have developed the system-size expan-

$$\begin{tikzcd}
\text{Langevin (State) Eq.} \arrow[r, "P"] \arrow[d, "E"'] & \text{Kalman Filter} \arrow[d, "E"] \\
\text{Non-Markovian Eq.} \arrow[r, "P"] & \text{AR-MA Model}
\end{tikzcd}$$

FIG. 1. Commutative diagram of manipulations. P denotes the projection of state variables onto the space spanned by observed quantities and E represents the elimination of irrelevant variables.

sion method using the scaling relation in order to obtain the asymptotic nature of a Markovian system far from equilibrium. Tomita and Tomita[3] have derived a linear Fokker-Planck equation for fluctuations in a normal scaling case. Since the linear Fokker-Planck equation can be transformed into an equivalent Langevin equation, let us begin by assuming that the system in a steady state is described by the linear Langevin equation

$$\frac{d}{dt}x(t)=Kx(t)+r(t)\ , \qquad (2)$$

where $x(t)$ is the fluctuation with $\langle x(t)\rangle=0$, and where the causality condition $\langle x(0)r^T(t)\rangle=0$ $(t>0)$ and the whiteness of the random force $\langle r(0)r^T(t)\rangle=D\delta(t)$ are assumed. The vector $x(t)$ is a d-dimensional state variable at time t, K the regression matrix, $r(t)$ the Gaussian white noise, D the diffusion matrix, and $\langle\ \cdots\ \rangle$ the ensemble average. The superscript T denotes transposition. The matrices K and D are related physically to elemental quantities such as the transition probabilities. The vector $x(t)$ must consist of a sufficient number of physical quantities so that the system is expressed by the Markovian process.

On the other hand, it is plausible from the practical limitation of data processing or of measurement in macroscopic systems that the complete set $x(t)$ of state variables consists of observable or known variables $y(t)$ and hidden variables $g(t)$. Since in this case the number of observable state variables is not enough for the Markovian description, the possible way for the description is that the information on unobservable variables can be equivalently expressed in terms of that contained in observed time-series data. So, in what follows in this paper, let us start with the assumption that data of observable variables are given.

By introducing the matrix $H=[I,0]$, where I is a q-dimensional unit matrix $(q<d)$, the contraction of information on hidden variables can be expressed by

$$y(t)=Hx(t)=[I,0]\begin{bmatrix}y(t)\\ g(t)\end{bmatrix}\ . \qquad (3)$$

It is easy to understand that the hidden variables make the basic equation non-Markovian as follows[15]:

$$\frac{d}{dt}y(t)=K_{11}y(t)+K_{12}\int_{t_0}^{t}\exp[(t-\tau)K_{22}]K_{21}y(\tau)d\tau+K_{12}\exp[(t-t_0)K_{22}]g(t_0)$$
$$+r_y(t)+\int_{t_0}^{t}K_{12}\exp[(t-\tau)K_{22}]r_g(\tau)d\tau\ , \qquad (4)$$

where

$$K=\begin{bmatrix}K_{11} & K_{12}\\ K_{21} & K_{22}\end{bmatrix}$$

and

$$r(t)=\begin{bmatrix}r_y(t)\\ r_g(t)\end{bmatrix}\ .$$

In this naive prescription, there remain ambiguities in the differences between the integration form (4) and the summation from (1), and in the appearance of the additional term $K_{12}\exp[(t-t_0)K_{22}]g(t_0)$. To avoid these difficulties, we now introduce another way of contraction of information and make the coarse graining in time. Integrating Eq. (2) from $(n-1)\Delta t$ to $n\Delta t$, we have [13]

$$x(n)=\Phi x(n-1)+f(n)\ , \qquad (5)$$

with $\langle f(n)\rangle=0$ and $\langle f(n)f^T(m)\rangle = V\delta_{nm}$, where δ_{nm} is the Kronecker's symbol and the coarse-grained variables are defined by

$$x(n)=x(n\Delta t)\ ,$$
$$\Phi=\exp(K\Delta t)\ ,$$
$$f(n)=\int_{(n-1)\Delta t}^{n\Delta t}\exp[K(n\Delta t-s)]r(s)ds\ ,$$
$$V=\int_0^{\Delta t}\exp(Ks)D\exp(K^Ts)ds\ .$$

The measurement equation (3) is also rewritten as

$$y(n)=Hx(n)\ , \qquad (6)$$

where $y(n)=y(n\Delta t)$. The framework of Eqs. (5) and (6) is called the state-space representation in control theory.

It is convenient to introduce a time-evolution operator z such that $zx(n)=x(n+1)$; then our basic equations [(5) and (6)] are

$$\begin{cases} zx(n)=\Phi x(n)+zf(n)\ ,\\ y(n)=Hx(n)\ . \end{cases} \qquad (7)$$

The direct relation between the input $f(n)$ and the output $y(n)$ is obtained by elimination of $x(n)$ from Eq. (7):

$$y(n)=G(z)f(n)\ , \qquad (8)$$

where $G(z)=H(zI-\Phi)^{-1}z$ is called the transfer function matrix. Formally expanding $G(z)$ in powers of z^{-1}, we can rewrite Eq. (8) as

$$y(n)=\sum_{i=0}^{\infty} W(i)f(n-i)\ , \tag{9}$$

which is an MA model of an infinite order, where $W(i)=H\Phi^i$ is the impulse response function. In order to obtain a time-series model of finite order, the rational matrix $G(z)$ must be decomposed into the $q\times q$ and $q\times d$ polynomial matrices

$$A(z)=\sum_{i=0}^{M} A_i z^{M-i}$$

and

$$B(z)=\sum_{i=0}^{L} B_i z^{M-i}\ ,$$

respectively, such that, $G(z)=A(z)^{-1}B(z)$. However, this decomposition is not unique. If we decompose $G_1(z)=A_1(z)^{-1}B_1(z)$, then we also have another decomposition $G_2(z)=A_2(z)^{-1}B_2(z)$, where $A_2(z)=Q(z)A_1(z)$ and $B_2(z)=Q(z)B_1(z)$ with any $q\times q$ nonsingular matrix $Q(z)$. Since the common factor $Q(z)$ cannot be uniquely determined in the identification of model from observed data, we consider it the most suitable, if $A(z)$ and $B(z)$ are polynomials of minimum degree in z. The decomposition form minimizing the degrees M and L has been studied in the realization problem of control and system theory. We now use the Luenberger method[16] to find the decomposition.

If Eq. (7) describing the system satisfies the condition of observability, we can choose d linearly independent column vectors from those of the matrix defined by

$$N=[H^T,\Phi H^T,\ldots,\Phi^{d-1}H^T]\ ,$$

where rank $N=d$. With these d-independent column vectors selected from N, we define a transformation matrix

$$T=[h_1,(\Phi^T)h_1,\ldots,(\Phi^T)^{\sigma_1-1}h_1,h_2,\ldots,(\Phi^T)^{\sigma_2-1}h_2,\ldots,h_q,\ldots,(\Phi^T)^{\sigma_q-1}h_q]^T\ ,$$

where $\sum_{i=1}^{q}\sigma_i=d$, h_i^T is the ith row vector of H, and σ_i is the Kronecker index which depends on the structure of Φ and H. Then, we can define a new state vector $x'(n)$ through the inverse matrix $S(=T^{-1})$ as

$$x(n)=Sx'(n)\ . \tag{10}$$

The basic equations are transformed into

$$\begin{cases} zx'(n)=\Phi'x'(n)+Tzf(z)\ ,\\ y(n)=H'x'(n)\ . \end{cases} \tag{11}$$

Here, the regression matrix is

$$\Phi'=T\Phi S=\begin{bmatrix}\Phi'_{11} & \cdots & \Phi'_{1q}\\ \vdots & & \vdots\\ \Phi'_{q1} & \cdots & \Phi'_{qq}\end{bmatrix}$$

with the submatrices

$$\Phi'_{ii}=\begin{array}{cl}\begin{bmatrix}0 & 1 & 0 & \cdots & 0\\ \vdots & & \ddots & \ddots & \vdots\\ & & & & 0\\ 0 & & \cdots & 0 & 1\\ a_{ii,\sigma_i} & & \cdots & & a_{ii,1}\end{bmatrix} & \sigma_i\text{rows},\\ \sigma_i\text{ columns} & \end{array}$$

$$\Phi'_{ij}=\begin{array}{cl}\begin{bmatrix}0 & \cdots & 0\\ \vdots & & \vdots\\ 0 & \cdots & 0\\ a_{ij,\sigma_j} & \cdots & a_{ij,1}\end{bmatrix} & \sigma_i\text{rows}\quad (i\neq j)\\ \sigma_j\text{ columns} & \end{array}$$

where $a_{ij,l}=h_i^T\Phi^{\sigma_i}s_{k_j-l+1}$ ($k_j=\sum_{i=1}^{j}\sigma_i$) and s_i is the ith column vector of S. The observation matrix H' is

$$H'=HS=\begin{array}{cl}\left[\begin{array}{cccc|cccc|c|cccc}1&0&\cdots&0&0&0&\cdots&0& &0&0&\cdots&0\\0&0&\cdots&0&1&0&\cdots&0& &0&0&\cdots&0\\0&0&\cdots&0&0&0&\cdots&0& &0&0&\cdots&0\\\vdots&\vdots& &\vdots&\vdots&\vdots& &\vdots&\cdots&\vdots&\vdots& &\vdots\\0&0&\cdots&0&0&0&\cdots&0& &0&0&\cdots&0\\0&0&\cdots&0&0&0&\cdots&0& &1&0&\cdots&0\end{array}\right] & q\text{ rows}\ .\\ \qquad\sigma_1\qquad\qquad\sigma_2\qquad\qquad\sigma_q\ \text{ columns} & \end{array}$$

As shown in Appendix A, observable variables satisfy

$$z^{\sigma_i}y_i(n)-\sum_{j=1}^{q}\sum_{l=1}^{\sigma_j}a_{ij,l}z^{\sigma_j-l}y_j(n)=\sum_{l=1}^{\sigma_i}h_i^T\Phi^{l-1}z^{\sigma_i-l+1}f(n)-\sum_{j=1}^{q}\sum_{k=1}^{\sigma_j-1}\sum_{l=0}^{k-1}a_{ij,\sigma_j-k}h_i^T\Phi^l z^{k-l}f(n)\ . \tag{12}$$

Comparing Eq. (12) with Eq. (8), we have

$$G(z)=A(z)^{-1}B(z)\ , \tag{13}$$

where $A(z)=[A_{ij}(z)]$, $B(z)=[b_1(z),\ldots,b_q(z)]^T$, and

$$A_{ij}(z)=z^{\sigma_i}\delta_{ij}-\sum_{l=1}^{\sigma_j}a_{ij,l}z^{\sigma_j-l}\quad(i,j=1,2,\ldots,q)$$

$$b_i(z)=\sum_{l=1}^{\sigma_i}h_i^T\Phi^{l-1}z^{\sigma_i-l+1}-\sum_{j=1}^{q}\sum_{k=1}^{\sigma_j-1}\sum_{l=0}^{k-1}a_{ij,\sigma_j-k}h_j^T\Phi^l z^{k-l}\quad(i=1,2,\ldots,q)\ .$$

By putting $M=\max(\sigma_i)$, we can symbolically rewrite $A(z)$ and $B(z)$ as

$$A(z)=\sum_{k=0}^{M}A_k z^{M-k}$$

and

$$B(z)=\sum_{k=0}^{M-1}B_k z^{M-k}\ .$$

Hence, it is concluded that, in the model with minimum orders, the degree L of $B(z)$ is $M-1$ when the degree of $A(z)$ is M. From the above algebraic transformation, we have a discrete non-Markov Langevin equation $A(z)y(n)=B(z)f(n)$:

$$\sum_{i=0}^{M}A_i y(n-i)=\sum_{i=0}^{M-1}B_i f(n-i)\ . \tag{14}$$

The coefficients A_i and B_i are uniquely determined by the structure of matrices Φ, H, and T. The structure of T depends on the selection of Kronecker index $\{\sigma_i\}$.

B. AR-MA model

Equation (14) is an AR-MA model in a wide sense: Statistical quantities of noise force $f(n)$, however, cannot be identified from observed data, while we assume that time-series data of observable variables are given in our formalism. It is necessary to further replace $f(n)$ by an equivalent quantity which generates the same output $y(n)$ and can be determined from the data. Such a quantity is called an innovation in time-series analysis. As will be shown in the remaining part of this section, the noise force in Eq. (14) can be expressed in terms of the innovation

$$\gamma(n)=y(n)-y(n\mid n-1)\ , \tag{15}$$

where $y(n\mid n-1)$ is the least-squares estimator, i.e., the most probable estimator under the condition that

$$Y(n-1)^T=[y(n-1)^T,y(n-2)^T,\ldots]$$

is given. When the system is in a normal case, the state variables possess the Gaussianity.[3,4] Hence, the value of estimator $y(n\mid n-1)$ can be evaluated by the Gaussian conditional mean value:

$$\begin{aligned}y(n\mid n-1)&=E\{y(n)\mid Y(n-1)\}\\&=\langle y(n)Y(n-1)^T\rangle\langle Y(n-1)Y(n-1)^T\rangle^{-1}Y(n-1)\ .\end{aligned}$$

Geometrically, $y(n\mid n-1)$ is the component of $y(n)$ orthogonally projected upon the linear manifold spanned by the vectors $Y(n-1)$.

By taking the conditional average $E\{\cdot\mid Y(n-1)\}$ of both sides of Eq. (14), we have

$$A_0y(n\mid n-1)+\sum_{i=1}^{M}A_i y(n-i)=\sum_{i=0}^{M-1}B_i f(n-i\mid n-1)\ , \tag{16}$$

where

$$f(k\mid m)=E\{f(k)\mid Y(m)\}$$
$$=\langle f(k)Y(m)^T\rangle\langle Y(m)Y(m)^T\rangle^{-1}Y(m)\ .$$

As mentioned in Appendix B, we can see that the projected noise force satisfies a recursion relation,

$$f(k\mid m)=VW(m-k)^T\Gamma(m)^{-1}\gamma(m)-\langle f(k)Y(m-1)^T\rangle\Theta(m)\gamma(m)+f(k\mid m-1)\ ,$$

where W is the impulse response function in Eq. (9), and Θ is defined by

$$\Theta(m)=\langle Y(m-1)Y(m-1)^T\rangle^{-1}\langle Y(m-1)y(m)^T\rangle\Gamma(m)^{-1}\ .$$

If we use the causality condition to truncate the recursion relation, we can obtain

$$f(k\mid m)=\sum_{i=0}^{m-k}R_k(m-i)\gamma(m-i)\ , \tag{17}$$

where

$$R_k(m-i)=VW(m-k-i)^T\Gamma(m-i)^{-1}-\langle f(k)Y(m-i)^T\rangle\Theta(m-i)\ .$$

Substituting Eq. (17) into Eq. (16), and rearranging the terms, we have

$$A_0y(n\mid n-1)+\sum_{i=1}^{M}A_iy(n-i)=\sum_{i=1}^{M-1}\sum_{j=0}^{i-1}B_iR_{n-i}(n-j-1)\gamma(n-j-1)\ . \tag{18}$$

We now obtain from Eqs. (15) and (18) the AR-MA−type equation:

$$A_0y(n)+\sum_{i=1}^{M}A_iy(n-i)=A_0\gamma(n)+\sum_{i=1}^{M-1}C_i\gamma(n-i)\ , \tag{19}$$

where

$$C_i=\sum_{l=i}^{M-1}B_lR_{n-l}(n-i)\ .$$

It is concluded that the system described by the Langevin equation with the observability condition has the AR-MA representation with the orders determined from the structure of matrices H' and Φ' in Eq. (11). The coefficients of AR-MA model have been related to the matrices of physical model (7).

Since Eq. (19) is a non-Markovian physical equation, we can expect a kind of fluctuation dissipation theorem between the coefficients A_i, B_i, C_i, and the new random forces. Comparing Eq. (19) with Eq. (14), we can find the relation between the physical random forces and the innovation forces:

$$A_0\gamma(n)+\sum_{i=1}^{M-1}C_i\gamma(n-i)=\sum_{i=0}^{M-1}B_if(n-i)\ .$$

By virtue of the whiteness of $f(n)$ and the orthogonal property of $\gamma(n)$, the evolution equation of innovation variance $\Gamma(n)=\langle\gamma(n)\gamma(n)^T\rangle$ is

$$A_0\Gamma(n)A_0^T+\sum_{i=1}^{M-1}C_i\Gamma(n-i)C_i^T=\sum_{i=0}^{M-1}B_iVB_i^T\ . \tag{20}$$

Since the steady variance of Eq. (5) for an aged system satisfies

$$\langle xx^T\rangle=\Phi\langle xx^T\rangle\Phi^T+V\ , \tag{21}$$

Eq. (20) provides the generalized Einstein relation

$$A_0\Gamma(\infty)A_0^T+\sum_{i=1}^{M-1}C_i\Gamma(\infty)C_i^T=\sum_{i=0}^{M-1}B_i(\langle xx^T\rangle-\Phi\langle xx^T\rangle\Phi^T)B_i^T\ . \tag{22}$$

III. CONTRACTION OF INFORMATION

A. Kalman filter

In Sec. II, the two operations have been performed on the basic equation (5): (i) elimination of the irrelevant variables, and (ii) projection on the observable variable space. It is interesting to note that another relationship is found between the physical state equation and the AR-MA model, when we change the order of the operations. By projecting the physical state equation on the observable space before eliminating the irrelevant variables, we will find an equation called a Kalman filter without observation noises in control theory. This procedure also gives the evolution equation of the residual of the state variables.

The state equation (5) is first transformed by taking the conditional average into

$$\begin{aligned} x(n\mid n-1) &= E\{x(n)\mid Y(n-1)\} \\ &= \Phi E\{x(n-1)\mid Y(n-1)\} \\ &= \Phi E\{x(n-1)\mid Y(n-2)\} + \Phi E\{x(n-1)\mid \gamma(n-1)\} \\ &= \Phi x(n-1\mid n-2) + \Phi P(n-1) H^T \Gamma(n-1)^{-1}\gamma(n-1)\,, \end{aligned} \tag{23}$$

where $\epsilon(n)=x(n)-x(n\mid n-1)$ is the residual of the state variables and $P(n)=\langle \epsilon(n)\epsilon(n)^T\rangle$. The projected equation (23) is easily rewritten as

$$x(n\mid n)=\Phi x(n-1\mid n-1)+F(n)\gamma(n)\,, \tag{24}$$

which is the Kalman filter[17] in control theory, where $F(n)=P(n)H^T\Gamma(n)^{-1}$.

Since we have the relation $\Gamma(n)=HP(n)H^T$ from the definition of the innovation $\gamma(n)$ and the residual $\epsilon(n)$, with $\Gamma(n)$ being evaluated by Eq. (20), we can find the evolution equation of $P(n)$. It follows from Eqs. (5) and (23) that

$$\epsilon(n)=\Phi\{I-F(n)H\}\epsilon(n-1)+f(n)\,.$$

If we square both sides of this equation and take an ensemble average, we obtain

$$\begin{aligned} P(n) &= \Phi\{I-F(n)H\}P(n-1)\{I-F(n-1)H\}^T\Phi^T+V \\ &= \Phi\{P(n-1)-P(n-1)H^T\Gamma(n-1)^{-1}HP(n-1)\}\Phi^T+V\,, \end{aligned} \tag{25}$$

which is the Riccati equation well known in the Kalman filter theory. Thus, it is concluded that Eq. (20) is closely related to the Riccati equation.

B. Markovian representation

As the manipulation of projection has been taken, let us next eliminate irrelevant variables. By taking the conditional average, the measurement equation (6) is projected as

$$y(n)=Hx(n\mid n)\,. \tag{26}$$

The difference between the physical basic equation (5) and Eq. (24) is that the noise force $f(n)$ in Eq. (5) is replaced in Eq. (24) by $F(n)\gamma(n)$. Since the canonical form of Luenberger, T, depends only on the matrices H and Φ involved in Eqs. (24) and (26), the matrix T is the same as that in the basic equations of Sec. II A. Therefore, we have for the variables $x'(n\mid n)=Tx(n\mid n)$,

$$x'(n\mid n)=\Phi' x'(n-1\mid n-1)+TF(n)\gamma(n)\,, \tag{27}$$

$$y(n)=H'x'(n\mid n)\,, \tag{28}$$

where Φ' and H' are the same as those in Eq. (11). Equation (27) is called the Markovian representation.[18]

Since the conditional average of $x(n+l)$ for $l\geq 1$ is

$$E\{x(n+l)\mid Y(n)\}=\Phi^l x(n\mid n)\,,$$

the state vector $x'(n\mid n)$ is rewritten by using the definition of the transformation matrix and the relation (26) as

$$x'(n\mid n)=\begin{bmatrix} h_1 \\ h_1\Phi \\ \vdots \\ h_1\Phi^{\sigma_1-1} \\ h_2 \\ \vdots \\ h_q\Phi^{\sigma_q-1}\end{bmatrix} x(n\mid n)=\begin{bmatrix} y_1(n) \\ y_1(n+1\mid n) \\ \vdots \\ y_1(n+\sigma_1-1\mid n) \\ y_2(n) \\ \vdots \\ y_q(n+\sigma_q-1\mid n)\end{bmatrix} \tag{29}$$

Then, an AR-MA—type equation may be derived by elimination of the estimators in Eqs. (27) and (28). However, this derivation is tedious, not lucid and complicated except when the ratio n/m of the dimension of the state variables and that of the observable variables is an integer. Therefore, let us derive, conversely, the Markovian representation from the AR-MA equation (see Fig. 2).

By taking the conditional average of both sides of the AR-MA equation (19), we have

$$\sum_{i=0}^{M} A_i y(n+M-i \mid n)=A(z)y(n \mid n)=0 , \quad (30)$$

where

$$zy(n \mid m)=y(n+1 \mid m) .$$

We can rewrite each component as

$$y_i(n+\sigma_i \mid n)=\sum_{j=1}^{q}\sum_{l=1}^{\sigma_j} a_{ij,l}y_j(n+\sigma_j-l \mid n) \quad (i=1,2,\ldots,q) \quad (31)$$

by using the expression $A_{ij}(z)$ in Eq. (13). The representation (29) and Eq. (31) provide us with the relation

$$x'(n+1 \mid n)=\Phi' x'(n \mid n) , \quad (32)$$

where Φ' has the canonical form of Luenberger. As the relation between the input $\gamma(n)$ and the output $y(n)$ of the AR-MA model (19) can be put as

$$y(n)=\sum_{j=0}^{\infty} W(j)\gamma(n-j) ,$$

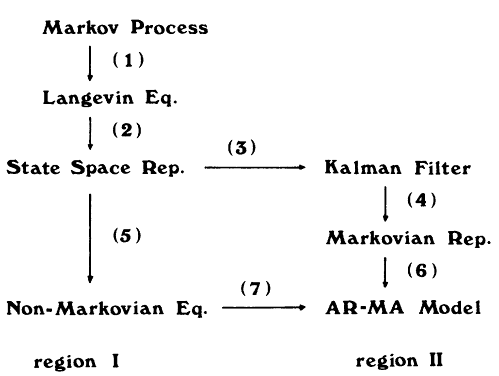

FIG. 2. Conceptual flow chart of contraction of information: (1) the system-size expansion method with a normal scaling relation in a steady state; (2) coarse graining in time; (3) mapping or projection from state space to observable space; (4) transformation by using the Luenberger canonical form in the minimum realization problem; (5) contraction of information on irrelevant variables; (6) transformation; (7) innovation process of noise force.

where the impulse response weights $W(j)$ satisfy the equations

$$A_0 W(0)=A_0 ,$$

$$A_0 W(j)+\sum_{i=1}^{j} A_i W(j-1)=C_j \quad \text{for } j=1,2,\ldots,M-1 ,$$

$$A_0 W(j)+\sum_{i=1}^{M} A_i(j-i)=0 \quad \text{for } j \geq M ,$$

we obtain from the orthogonal property of $\gamma(n)$ the relation

$$y(n+i+1 \mid n+1)=y(n+i+1 \mid n) + W(i)\gamma(n+1) ,$$

which is rewritten in the vector form as

$$x'(n+1 \mid n+1)=x'(n+1 \mid n)+G\gamma(n+1) . \quad (33)$$

Combining Eqs. (32) and (33), we have the Markovian representation of the AR-MA model

$$x'(n+1 \mid n+1)=\Phi' x'(n \mid n)+G\gamma(n+1) , \quad (34)$$

where G is defined by

$$G_{ij}=W_{\rho j}(l)$$

for $l=i-k_{\rho-1}-1$ and $i,j=1,2\ldots,q$.

Comparing Eq. (34) with Eq. (27), we can find that G is equal to $TF(n+1)$. This is because the linear equations have the same coefficient matrix Φ', and they possess the same input and output.

C. Contraction of information

We can summarize our formalism in Fig. 2 (Ref. 19): The irrelevant variables have been eliminated to derive macroscopic non-Markovian equations as in the statistical physics.[5,6] After this manipulation, the state variables have been projected on the space spanned by observed quantities to derive the time-series models. Since the basic equations for a finite dimensional system are linear, the two manipulations are commutative as shown in Fig. 1; that is, $P \cdot E$ (Langevin Eq.)$=E \cdot P$ (Langevin Eq.) = AR-MA model. The order of the manipulations is, however, important. If we change the order of manipulations, we can derive the Kalman filter in the control theory as seen above. Therefore, this schematic diagram of Fig. 1 is essential to understand the contraction of information in macroscopic systems. Furthermore, the noncommutativity, $[E,P]=E\cdot P-P\cdot E\neq 0$, will become important in a non-normal or a nonstationary case, where nonlinear effects cannot be neglected. In the nonlinear case, the physical way $P\cdot E$ is not the same as the control or mathematical way $E\cdot P$.

From the viewpoint of the contraction of information, it should be noted that there are two kinds of Markovian equation in Figs. 1 or 2: The equation (24) of Markovian representation determined from the AR-MA model has the noise term different from that in the original Markovian or physical state expression (5), even if the time-series model is obtained so as to properly identify the system. Since the eigenvalues of the regression matrix are conserved in the Luenberger transformation, the dynamical property of the original system and the statistical property of the observable variables can be reproduced by incorporating the time-series data of the observable variables instead of the eliminated variables. The reproduction is, however, not complete for the total system. We lose the information by the contraction or projection. From this viewpoint, it should be noted in Fig. 2 that the stochastic state vector $x(n)$ plays an important role in the region I including the state-space representation and the non-Markovian Langevin equation, and that the conditional state expectation $x(n\mid n-1)$ plays a dominant role in the region II including the Kalman filter, the Markovian representation, and the AR-MA model. Therefore, let us consider the change of information between the probability and the conditional probability, which may be represented by

$$\begin{aligned} I_n &= -\int P\{x(n)\}\ln P\{x(n)\}dx(n)+\int P\{x(n),Y(n-1)\}\ln P\{x(n)\mid Y(n-1)\}dx(n)dY(n-1) \\ &= \int P\{x(n),Y(n-1)\}\ln\frac{P\{x(n)\mid Y(n-1)\}}{P\{x(n)\}}dx(n)dY(n-1) \\ &= E\left\{\ln\frac{P\{x(n)\mid Y(n-1)\}}{P\{x(n)\}}\right\} . \end{aligned} \tag{35}$$

This quantity, which is called a mutual information, is interpreted as the difference between information in the physical model and that in the time-series model. The normality of the system guarantees Eq. (35) to be transformed into

$$\begin{aligned} I_n &= \tfrac{1}{2}\ln\{\det[\Sigma(n)P(n)^{-1}]\} \\ &\quad +\tfrac{1}{2}E\{x(n)^T\Sigma(n)^{-1}x(n)\}-\tfrac{1}{2}E\{[x(n)-x(n\mid n-1)]^TP(n)^{-1}[x(n)-x(n\mid n-1)]\} \\ &= \tfrac{1}{2}\ln\{\det[\Sigma(n)P(n)^{-1}]\} , \end{aligned} \tag{36}$$

where $\Sigma(n)=\langle x(n)x(n)^T\rangle$. In the steady system, the mutual information is expressed by

$$I=\tfrac{1}{2}\ln\{\det[\Sigma(\infty)P(\infty)^{-1}]\} . \tag{37}$$

Finally, it is worthwhile to interpret the change of information as follows: Since I_n can be written as

$$\begin{aligned} I_n &= -\int P\{x(n)\}\ln P\{x(n)\}dx(n)+\int P\{x(n),Y(n-1)\}\ln P\{x(n)\mid Y(n-1)\}dx(n)dY(n-1) \\ &= -\int \langle\langle P\{x(n)\mid Y(n-1)\}\rangle\rangle\ln\langle\langle P\{x(n)\mid Y(n-1)\}\rangle\rangle dx(n) \\ &\quad +\int \langle\langle P\{x(n)\mid Y(n-1)\}\ln P\{x(n)\mid Y(n-1)\}\rangle\rangle dx(n) \\ &= -\int (H[\langle\langle P\{x(n)\mid Y(n-1)\}\rangle\rangle]-\langle\langle H[P\{x(n)\mid Y(n-1)\}]\rangle\rangle)dx(n) , \end{aligned} \tag{38}$$

where $H[\cdot]=[\cdot]\ln[\cdot]$ and $\langle\langle \cdots \rangle\rangle=\int dY(n-1)\cdots P\{Y(n-1)\}$. The mutual information corresponds to the noncommutativity of $H[\cdot]$ and $\langle\langle \cdots \rangle\rangle$.

IV. A SIMPLE EXAMPLE

Let us examine a system with two degrees of freedom to illustrate the present theory briefly. The physical equations [(5) and (6)] are summarized as

$$\begin{bmatrix} x_1(n) \\ x_2(n) \end{bmatrix} = \Phi \begin{bmatrix} x_1(n-1) \\ x_2(n-1) \end{bmatrix} + \begin{bmatrix} f_1(n) \\ f_2(n) \end{bmatrix} \tag{39}$$

and

$$y(n) = (1\ 0) \begin{bmatrix} x_1(n) \\ x_2(n) \end{bmatrix} , \tag{40}$$

with a steady variance σ of Eq. (21)

$$\sigma = \phi \sigma \phi^T + v , \tag{41}$$

where

$$\phi = \begin{bmatrix} \omega & 1 \\ -1 & 1-\omega \end{bmatrix} , \quad v = \begin{bmatrix} v_{11} & v_{12} \\ v_{12} & v_{22} \end{bmatrix} , \quad \text{and} \quad \sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix} .$$

The canonical form of Leunberger is defined as

$$T = \begin{bmatrix} 1 & 0 \\ \omega & 1 \end{bmatrix} \quad \text{and} \quad S = \begin{bmatrix} 1 & 0 \\ -\omega & 1 \end{bmatrix} ,$$

and then the AR-MA model (19) becomes

$$y(n) - y(n-1) + (-\omega^2 + \omega + 1) y(n-2) = \gamma(n) + \alpha \gamma(n-1) , \tag{42}$$

with the evolution equation (20) of the innovation variance

$$\sigma_{\gamma\gamma}(n) + \frac{\beta_1}{\sigma_{\gamma\gamma}(n-1)} = \beta_2 , \tag{43}$$

where

$$\alpha = \{ (\omega - 1) v_{11} + v_{12} \} / \sigma_{\gamma\gamma}(n-1) ,$$

$$\beta_1 = \{ (\omega - 1) v_{11} + v_{12} \}^2 ,$$

$$\beta_2 = (\omega^2 - 2\omega + 2) v_{11} + (\omega - 1) v_{12} + v_{22} .$$

From Eq. (27) or (34), the Markovian representation of the AR-MA model is also expressed as

$$\begin{bmatrix} y(n) \\ y(n+1 \mid n) \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ \omega^2 - \omega - 1 & 1 \end{bmatrix} \begin{bmatrix} y(n-1) \\ y(n \mid n-1) \end{bmatrix} + \begin{bmatrix} 1 \\ \alpha + 1 \end{bmatrix} \gamma(n) . \tag{44}$$

When a two-dimensional system is properly identified as the time-series model (42) by using a suitable information criterion, we can see the following.

(i) The time-series model we have found is the AR-MA type, and not the AR type.
(ii) The AR order M of the time-series model (19) is 2 and the MA order L is 1.
(iii) The coefficients in AR and MA terms are

$$A_1 = -\mathrm{tr}\Phi = -1, \quad A_2 = \det\Phi = -\omega^2 + \omega + 1, \quad \text{and} \quad C_1 = \frac{-\phi_{22} v_{11} + \phi_{12} v_{12}}{\sigma_{\gamma\gamma}} = \alpha .$$

These relations are uniquely determined, since the number of observable variables is one.

(iv) In Eqs. (39), (42), and (44) eigenvalues are common, so that the dynamical properties are con-

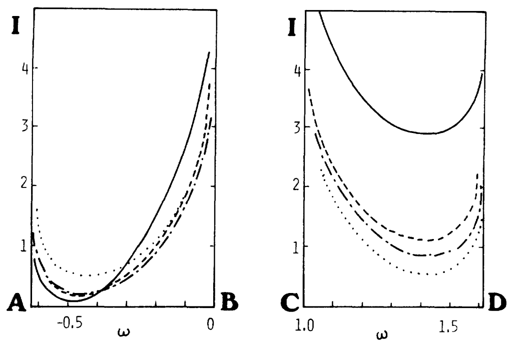

FIG. 3. Mutual information on contraction of information. Lines AB and CD are stable regions, where parameters are $V=V_0\left(\begin{smallmatrix}1 & b\\ b & a\end{smallmatrix}\right)$, $V_0=100$, and (a,b) — — — — —for (1.0, 0.5), — - — -for(1.0, 0.05), ——for (0.01, 0.05), ---------- for (25.0, 0.5).

served.

Finally, let us treat numerically the contraction of information as follows: When the value ω is treated as a parameter of a dynamical system, the stable regions are determined from the linear stability criterion. The stable regions are $(1-\sqrt{5})/2<\omega<0$ and $1<\omega<(1+\sqrt{5})/2$ as shown in the abscissas of Fig. 3. Both the ends of lines AB and CD are instability points.[20] The two points B and C represent the hard-mode instabilities. The other A and D are the soft-mode instability points. The solution of variance equation (41) is given by

$$\sigma=\sum_{i=0}^{\infty}\phi^i v(\phi^T)^i\,, \tag{45}$$

and increases divergently as ω approaches a value corresponding to the ends of each axis. In contrast to σ, the variance of innovation smoothly varies without divergence. Therefore, the mutual information has the same pattern as that of variance as seen from Eq. (37). The quantity I is shown in Fig. 3, where the determinant of $P(\infty)$ in the Riccati Eq. (25) is given by

$$\det P(\infty)=\{(1-\omega)^2 v_{11}-2(1-\omega)v_{12}+v_{22}\}\sigma_{\gamma\gamma}(\infty)$$
$$-\{(1-\omega)v_{11}-v_{12}\}^2\,.$$

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APPENDIX A

To obtain Eq. (12), the state vector is subdivided as

$$x'(n)=\begin{bmatrix}x_1'(n)\\ \vdots\\ x_q'(n)\end{bmatrix},$$

where each component is

$$x_i'(n)=\begin{bmatrix}x_{i,1}'(n)\\ \vdots\\ x_{i,\sigma_i}'(n)\end{bmatrix}=\begin{bmatrix}x_{k_{i-1}+1}'(n)\\ \vdots\\ x_{k_i}'(n)\end{bmatrix}\quad(i=1,2,\ldots,q)\,.$$

Then, Eq. (11) is expressed in terms of the components as

$$\begin{cases} zx_i'(n)=\sum_{j=1}^{q}\Phi_{ij}'x_j'(n)+T_i zf(n)\\ y_i(n)=x_{i,1}'(n)=x_{k_{i-1}+1}'(n)\end{cases}\quad(i=1,2,\ldots,q)$$

where $T_i^T=[h_i,\Phi^T h_i,\ldots,(\Phi^T)^{\sigma_i-1}h_i]$. Furthermore, the first equation of above state-space representation is rewritten as

$$\begin{cases} zx_{i,j}'(n)=x_{i,j+1}'(n)+h_i^T\Phi^{j-1}zf(n)\quad(j=1,2,\ldots,\sigma_i-1)\\ zx_{i,\sigma_i}'(n)=\sum_{j=1}^{q}\sum_{l=1}^{\sigma_j}a_{ij,l}x_{j,\sigma_j+1-l}(n)+h_i^T\Phi^{\sigma_i-1}zf(n)\,.\end{cases}$$

Eliminating the state variables except those identical with observable variables, we can have Eq. (12).

APPENDIX B

In this appendix we represent the conditional random force $f(\cdot\mid\cdot)$ in terms of the innovation $\gamma(\cdot)$. The causality condition and Eq. (9) give the relation

$$\langle f(k)Y(m)^T\rangle = \begin{cases} 0 \quad (k>m) \\ V[W(m-k)^T, W(m-k-1)^T,\ldots,W(0)^T,0\ldots] \quad (k\le m) \end{cases}.$$

The inverse of the covariance matrix of $Y(m)$ is given[13] by

$$\langle Y(m)Y(m)^T\rangle^{-1} = \begin{bmatrix} \langle y(m)y(m)^T\rangle & y(m)Y(m-1)^T\rangle \\ \langle Y(m-1)y(m)^T\langle & \langle Y(m-1)Y(m-1)^T\rangle \end{bmatrix}^{-1} = \begin{bmatrix} \Gamma(m)^{-1} & -\Theta(m) \\ -\Theta(m)^T & \Psi(m) \end{bmatrix},$$

where

$$\Gamma(m) = \langle \gamma(m)\gamma(m)^T\rangle$$
$$= \langle y(m)y(m)^T\rangle - \langle y(m)Y(m-1)^T\rangle\langle Y(m-1)Y(m-1)^T\rangle^{-1}\langle Y(m-1)y(m)^T\rangle$$
$$\Theta(m) = \langle Y(m-1)Y(m-1)^T\rangle^{-1}\langle Y(m-1)y(m)^T\rangle\Gamma(m)^{-1}$$
$$\Psi(m) = \Theta(m)\langle y(m)Y(m-1)^T\rangle\langle Y(m-1)Y(m-1)^T\rangle^{-1} + \langle Y(m-1)Y(m-1)^T\rangle^{-1}.$$

By using the above relations and writing as $Y(m)^T = [y(m)^T, Y(m-1)^T]$, we see that the projected noise force satisfies the recursion relation,

$$\begin{aligned} f(k\mid m) &= VW(m-k)^T\Gamma(m)^{-1}\{y(m) - \langle y(m)Y(m-1)^T\rangle\langle Y(m-1)Y(m-1)^T\rangle^{-1}Y(m-1)\} \\ &\quad - \langle f(k)Y(m-1)^T\rangle\Theta(m)\{y(m) - \langle y(m)Y(m-1)^T\rangle\langle Y(m-1)Y(m-1)^T\rangle^{-1}Y(m-1)\} \\ &\quad + f(k\mid m-1) \\ &= VW(m-k)^T\Gamma(m)^{-1}\gamma(m) - \langle f(k)Y(m-1)^T\rangle\Theta(m)\gamma(m) + f(k\mid m-1). \end{aligned}$$

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