

“Thermodynamics” from Time Series Data Analysis

Hiroshi Hasegawa*, Takashi Washio⁺ and Yukari Ishimiya*

Department of Mathematical Science, Ibaraki University*
I.S.I.R., Osaka University⁺

Abstract

We propose a derivation of statistical laws from time series data analysis on the analogy of the thermodynamics. Recently, Sekimoto and Sasa reconstructed thermodynamics of systems, which are governed by the Langevin equations. We construct “thermodynamics” by applying their approach to the Auto Regressive type models, in which the random fluctuation is no more thermal one. Since the detailed balance is broken in such system, irreversible circulation of fluctuation appears. We apply our arguments to the zero-power point reactor kinetics model. We try to derive new “thermodynamical” laws from actually data observed in a test nuclear reactor.

1 Introduction

Following the development of computer science, we have got a lot of knowledge from the analysis of huge numerical data. It is good chance to discover new science using this huge knowledge. In this paper, we propose a derivation of new statistical laws from time series data analysis. Our approach is based on the combination of theory of the time series data analysis and the effective theory for complex systems.

In the time series data analysis, the Auto Regressive (AR) type models are highly developed[1][2]. The many AR type models, Auto Regressive Moving Average (ARMA) model, Vector Auto Regressive model, Continuous Time ARMA model etc. have been proposed for the last twenty years[3]. Nonlinear models are also done, recently[4]. The AR type models work in many fields such as control of power plant, analysis of earthquake, price of stock market, etc.

In this paper, we consider the AR type models as effective theories for these complex systems. The effective theory is closed among macro or slow variables. We obtain it by integrating out the micro or fast variables. The theory of the Langevin equation is a typical effective theory, in which the effects from fast variable are treated as white noise. The coupled discretized Langevin equations govern the AR type models. We assume that the white noise in the AR type model is not measurement error and the effects of the underlying fast variables.

Recently, Sekimoto and Sasa reconstructed thermodynamics in a model of molecular machinery[5] governed by Langevin equation[6][7]. They interpreted the Langevin equation as balance one of forces and heat as work by reaction force to the heat bath. They derived the well-known thermodynamical laws, the first, the second and the Fourier law.

In this paper, we construct “thermodynamics” by applying Sekimoto-Sasa theory to the Auto Regressive type models for systems such as economical and biological ones, in which the random fluctuation is no more thermal. “Temperature” for noise source is associated with the strength of the random fluctuation. The time derivative is caused by “force”. Then, “thermodynamical” laws, “energy” conservation, positive “entropy” production and flow in proportion to “temperature” difference, appear with complete new interpretations in terms of economy and biology.

Since the detailed balance is broken in such systems, irreversible circulation of fluctuation appears[8][9]. We apply our arguments to the zero-power point reactor kinetics model[10]. We try to derive new “thermodynamical” laws from actually observed data from a test nuclear reactor.

In the section 2, we emphasize the importance of the effective theory for the discovery science. And we mentioned the relations among effective theories, such as thermodynamics and the theory of the Langevin equation. In the section 3, we draw the outline of Sekimoto-Sasa theory. In the section 4, we discuss about the braking of detailed balance in non-physical systems and irreversible circulation of fluctuation. In the section 5, we apply Sekimoto-Sasa theory the zero-point power reactor kinetics model. In the last section, we mention the application to the actual time

series data from a test nuclear power plant.

2 Relations among Effective Theories

If we know the fundamental laws of nature, which govern elementary particles, we could explain everything in nature, in principle. Scientists believed the reductionism for long times. Development of Science has been based on this concept.

Now, we need new picture of nature. We already know that there are many laws in complex systems. The details of the underlying microlevel dynamics do not affect the laws in macrolevel. The effects from microscale variables can be absorbed to parameters in macrolevel in some effective theory. These effective theories are called renormalizable one, which are developed in the elementary particle physics. The renormalizable theory, gauge field theory in the elementary particles physics, is typical effective theory. To understand the diversity of nature, we need the picture of effective theory.

Roughly speaking, there are two kinds of the effective theories. One is based on the separation between macro scale and micro one with respect to space or number of elements. The other one is with respect to time.

The typical example of the former is thermodynamics. The thermodynamic relations among state variables, whose order is $10^2 \sim 10^3$, are universal so not affected by each behavior of an element. For nuclei and polymers, in which the order of the number of elements are $10^2 \sim 10^3$, theory of collective coordinates are useful[11]. Since the separation is not complete, the interactions between two scales are treated as perturbation. When scaling exists from micro scale to macro one, for example, in the case of the second order phase transition, the renormalization theory is applicable [12].

On the other hand, the typical example of the latter is theory of Langevin equations, in which the correlation time is approximately neglected in comparison with the observation time. As we mentioned in the introduction, we consider the AR type model as an effective theory in the latter case. When long time correlation characterized by $1/f$ noise exists, adiabatic perturbation theory is useful [13].

Recently, we start understanding relations among the effective theories mentioned above. Sekimoto and Sasa reconstructed thermodynamics in a model of molecular machines governed by Langevin equation[6][7]. Oono discussed the relation between adiabatic perturbation theory and renormalization group theory[13].

3 Sekimoto–Sasa Theory

3.1 Outline of Sekimoto–Sasa Theory

In this section, we show the outline of Sekimoto–Sasa theory. For the detail, we mention Ref.[6] and Ref. [7].

Let us consider two particles and two heat bathes system. The particle 1 and 2 are coupled with the heat bath 1 and 2, respectively. The particle 1 and 2 are also connected by spring and the spring coefficient $a(t)$ can change in time. The system is governed by the following coupled Langevin equations,

$$\begin{aligned}\dot{x}_1 &= -a * (x_1 - x_2) + \xi_1(t) \\ \dot{x}_2 &= -a * (x_2 - x_1) + \xi_2(t)\end{aligned}$$

where x_1 and x_2 are position of the particle 1 and 2, respectively. $\xi_1(t)$ and $\xi_2(t)$ are thermal noises from the heat bath 1 and 2, respectively. The thermal noises are white as,

$$\begin{aligned}<\xi_1(t)\xi_1(t')> &= 2T_1\delta(t-t') \\ <\xi_2(t)\xi_2(t')> &= 2T_2\delta(t-t').\end{aligned}$$

In Sekimoto–Sasa theory, we interpret as follows, (1)Langevin equations are balance ones of forces. (2)Heat is work by reaction force to the heat bath.

Then, we can derive the conservation law of energy or the fast law,

$$\begin{aligned}<Q_1> + <Q_2> + a(t)* <(x-y)^2>/2 |_0^t \\ &= \int_0^t dt \dot{a}(t) * <(x-y)^2>/2\end{aligned}$$

where the first term of the left hand side , $<Q_1>$, and the second one, $<Q_2>$, are the heat to the heat bath 1 and the heat to the heat bath 2, respectively. The third one is the change of the potential energy from the change of the distance between the two particles. The right hand side is the work by the change of the parameter $a(t)$.

In the case of the constant parameter, $da(t)/dt = 0$, the Fourier law is valid so that the heat $<Q_1>$ and the heat $<Q_2>$ are proportional to the difference of the temperatures between the two heat bathes,

$$<Q_1> = <Q_F> \propto T_1 - T_2.$$

In the case of the slowly varying parameter, we can expand the heat $<Q_1>$ with respect to $da(t)/dat$,

$$<Q_1> = <Q_F> + <Q_R> + <Q_{IR}> + \dots$$

The new terms, reversible heat production $<Q_R>$ and irreversible heat production $<Q_{IR}>$, are proportional to $da(t)/dat$. The reversible heat production $<Q_R>$ is function of the initial parameter and the final one

and is not depend on the process. Therefore the reversible heat production $\langle Q_R \rangle$ exists even in quasistatic process. The irreversible heat production $\langle Q_{IR} \rangle$ is depend on the process. It vanishes in quasistatic process.

Sekimoto and Sasa showed the positivity of the irreversible heat production,

$$\langle Q_{IR} \rangle \geq 0$$

This result is known as the second law of thermodynamics.

As we showed, Sekimoto and Sasa reconstructed thermodynamics in the system governed by the coupled Langevin equations and derived the thermodynamic laws such as the first, the second and Fourier law.

3.2 What is Importance of Sekimoto–Sasa Theory

We emphasize why Sekimoto–Sasa theory is important. At first glance, they just reconstructed the well-known thermodynamics. After carefully checking their derivation, we notice that their derivation is only based on the coupled Langevin equations. By introducing the two interpretations about the balance equation and the heat, Sekimoto and Sasa recreated key concepts of energy and entropy.

This means that it is possible to construct “thermodynamics” in systems, which do not have to do with the real energy and heat. Associating with the strength of the random fluctuation, we may introduce “temperature” for noise sources. The time derivative is caused by “force”. Then, “thermodynamical” laws, “energy” conservation, positive “entropy” production and flow in proportion to “temperature” difference, appear with complete new interpretations.

For example, in economical systems, we may construct econo-thermodynamics with new words of econo-temperature and econo-force. Then, econo-thermodynamical laws, econo-energy conservation, positive econo-entropy production and flow in proportion to econo-temperature difference, appear with complete new interpretations.

We expect to be able to create new concepts by applying Sekimoto–Sasa theory to a system, which is governed by Langevin type equation. In general, the detailed balances are broken in systems such as economical or biological ones. The Boltzmann equilibrium distribution is no more steady state solution of the coupled Langevin equations, which breaks the detailed balances. We will discuss how to solve this problem in the next section.

4 Breaking of Detailed Balance and Irreversible Circulation of Fluctuation

We consider the model discussed in the previous section, again. To make situation simple, the both heat bathes have the same temperature T . To

discuss the breaking of the detailed balance, the force to x_1 is difference from one to x_2 so that the law of action and reaction is broken. Then, the coupled Langevin equations are given as,

$$\dot{x} = -a * (x - y) + \xi_1(t)$$

$$\dot{y} = +b * (x - y) + \xi_2(t).$$

The time evolution of the probability density $P(\mathbf{x}, t)$ is governed by the following Fokker–Plank equation,

$$\partial P(\mathbf{x}, t) / \partial t = \nabla \cdot [A\mathbf{x} + T\nabla] P(\mathbf{x}, t)$$

where the vector $\mathbf{x} = (x_1, x_2)$ and the elements of the matrix A is given as, $A_{1,1} = -A_{1,2} = -a$, $A_{2,1} = -A_{2,2} = b$. The matrix A is no more symmetric because of the breaking of the detailed balances, $A_{1,2} \neq A_{2,1}$.

By decomposing the matrix A into symmetric one \bar{A} and anti-symmetric one,

$$\begin{aligned} \partial P(\mathbf{x}, t) / \partial t &= (a - b)/2 * (x_1 \partial / \partial x_2 - x_2 \partial / \partial x_1) P(\mathbf{x}, t) \\ &\quad + \nabla \cdot [\bar{A}\mathbf{x} + T\nabla] P(\mathbf{x}, t). \end{aligned}$$

Notice that $R = x_1 \partial / \partial x_2 - x_2 \partial / \partial x_1$ is the generator of rotation.

In the rotating frame, $\tilde{\mathbf{x}} = \exp[(a - b)/2 * R * t]\mathbf{x} \exp[-(a - b)/2 * R * t]$, the Fokker–Plank equation is rewritten as

$$\partial P(\tilde{\mathbf{x}}, t) / \partial t = \nabla \cdot [\bar{A}\tilde{\mathbf{x}} + T\nabla] P(\tilde{\mathbf{x}}, t).$$

Effectively, the anti-symmetric part disappears so that the probability density $P(\tilde{\mathbf{x}}, t)$ approaches to the Boltzmann equilibrium distribution $P_{eq}(\tilde{\mathbf{x}})$,

$$P_{eq}(\tilde{\mathbf{x}}) = \exp[-U(\tilde{\mathbf{x}})/T]$$

where the effective potential energy $U(\tilde{\mathbf{x}}) = \tilde{\mathbf{x}} \cdot \bar{A}\tilde{\mathbf{x}}/2$.

In the original frame, the probability density rotates in time,

$$P(\mathbf{x}, t) = \exp[(a - b)/2 * R * t] \exp[-U(\mathbf{x})/T] \exp[-(a - b)/2 * R * t]$$

This is known as irreversible circulation of fluctuation [8][9]. In the irreversible circulation of fluctuation, noise plays an important role. Without noise, the probability density does not rotate and exponentially approaches to the origin $\mathbf{x} = \mathbf{0}$. The exponential decay is given as superposition of two independent eigenmodes. The two eigenvectors are not orthogonal each other, because of the asymmetry. When noise turns on, this breaks the symmetry between clockwise rotation and anti-clockwise one. The mechanism is analogous to the ratchet model introduced in molecular machinery [5].

In this section, we have shown that Sekimoto–Sasa theory is still applicable to a system, which is governed by Langevin equation with breaking detailed balance, in the frame of the certain rotation. Since the detailed balances are broken in economical or biological systems, we can expect to observe the irreversible circulation of fluctuation in these systems.

In the next section, we will discuss about point reactor kinetics model. Using this model we try to apply Sekimoto-Sasa theory to AR type model which is derived from actual time series data observed from test nuclear reactor.

5 Application to Zero-Power Point Reactor Kinetics Model

As the first trial, we apply our arguments in the previous section to zero-power point reactor kinetics model [?]. The reasons are as follows;(1)AR type models well work in the control of nuclear reactor. (2)To analyze test nuclear reactor is easier, since effective degree is smaller.(3)Linear approximation is typical for zero-power point reactor.(4) Quantum fluctuations, which play important rolls in the decay of nuclei , can be treated as white noise, in principle.(5)Instead of thermal fluctuations, we may derive new “thermodynamics” for quantum fluctuations.

The zero-power point reactor kinetics model is governed by the following coupled Langevin type equations,

$$dn/dt = (\rho - \beta)/\Lambda * n + \sum_i \lambda_i C_i + \xi_0(t)$$

$$dC_i/dt = \beta_i/\Lambda * n - \lambda_i C_i + \xi_i(t) \quad i = 1, \dots, 6$$

where n : concentration of neutron, C_i : concentration of i -th precursor, $\beta = \sum \beta_i$: rate of total delayed neutron, Λ : lifetime of prompt neutron, λ_i : decay constant of i -th precursor, ρ : reactivity.

We can expect that inverse of the lifetime of prompt neutron is much greater than decay constant of advanced nuclei, $\beta/\Lambda \gg \lambda_i$ and the ratio of total delayed neutron is much greater than the reactivity, $\beta \gg \rho$.

For the noise $\xi_i(t) = 0$, the time evolution of system is superposition of the following seven eigenmodes,

- (1) For one extremely fast exponentially decaying eigenmode, the eigenvalue $\sim O(\beta\lambda/\Lambda) * \lambda$.
- (2) For five exponentially decaying eigenmodes, the eigenvalues $\sim O(1) * \lambda$.
- (3)For one extremely slow exponentially decaying or growing eigenmode, the eigen value $\sim O(\rho/\beta) * \lambda$.

Steadystate of the nuclear reactor is corresponding to the last eigenmode. By adjusting the reactivity ρ , the power of the nuclear reactor is approximately kept constant.

For the noise $\xi_i(t) \neq 0$, we expect as follows;

- (1) The extremely fast exponentially decaying eigenmode almost decays out.
- (2) Among the five exponentially decaying eigenmodes, the irreversible circulation of fluctuations appears.
- (3)For the direction of the extremely slow exponentially decaying or growing eigenmode, the diffusion appears.

The extremely slow exponentially decaying or growing eigenmode can be approximated as linear decaying or growing mode. We can treat this mode as motion of center mass of the system. Therefore, we can apply Sekimoto-Sasa theory in the frame of certain rotation and the center mass, for which potential energy and Boltzmann equilibrium distribution can be defined.

6 Conclusions and Remarks

We propose a derivation of statistical laws from time series data analysis on the analogy of the thermodynamics. We construct “thermodynamics” by applying their approach to the Auto Regressive type models, in which the random fluctuation is no more thermal one. Since the detailed balance is broken, irreversible circulation of fluctuation appears. We apply our arguments to the zero-power point reactor kinetics model. We are trying to derive new “thermodynamical” laws from actually observed data from a test nuclear reactor.

In this paper, we consider the AR type models as effective theories. The theory of the Langevin equation is a typical effective theory, in which the effects from fast variable are treated as white noise. The coupled discretized Langevin equations govern the AR type models. We assume that the white noise in the AR type model is not measurement error and the effects of the underlying fast variables.

Sekimoto-Sasa theory derived thermodynamics of systems, which are governed by the Langevin equations. They interpreted the Langevin equation as balance one of forces and heat as work by reaction force to the heat bath. Thermodynamical laws, the first, the second and the Fourier law, were derived.

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We have shown that Sekimoto-Sasa theory is still applicable to a system, which is governed by Langevin equation with breaking detailed balance, in the frame of the certain rotation. Since the detailed balances are broken in economical or biological systems, we can expect to observe the irreversible circulation of fluctuation in these systems.

We apply our arguments to the zero-power point reactor kinetics model. Since one eigenmode is slowly growing or decaying approximately linearly, we need the center mass frame to apply the theory.

We are trying to derive new “thermodynamical” laws from actually observed data from a test nuclear reactor. We are planning to apply our arguments to some economical and biological systems.

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