

Stochastic thermodynamics of information

NCTS 2018 winter school

-Frontiers of complex systems science: soft matters, statistical physics, and big data

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Introduction

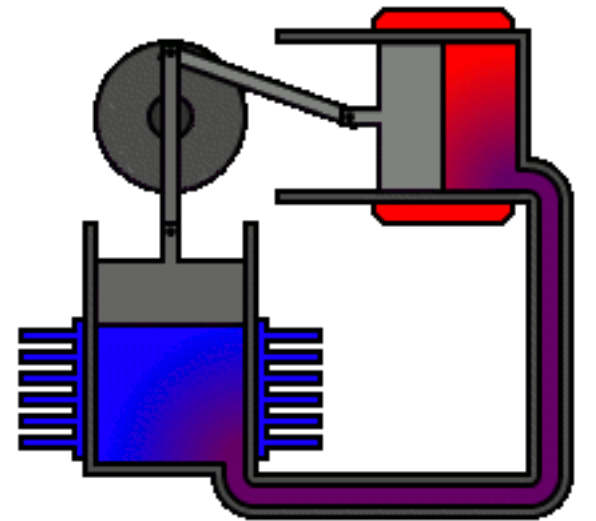
Introduction

Conventional thermodynamics

The system is macroscopic. (e.g., the gas in the box)

Dynamics are deterministic.

The interaction between two systems is negligible. (Additivity)



Stochastic thermodynamics

Textbook, Review

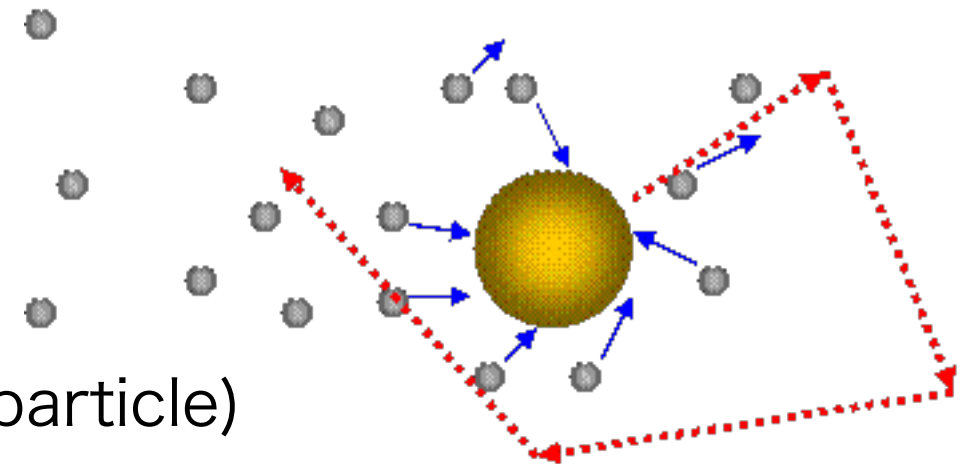
Sekimoto, K. (2010). *Stochastic energetics* (Vol. 799). Springer.

Seifert, U. (2012). *Reports on Progress in Physics*, 75(12), 126001.

The system is mesoscopic. (e.g., the Brownian particle)

Dynamics are stochastic. (Thermodynamic quantity is random variable.)

The interaction between two systems is NOT negligible. (Non-additivity)



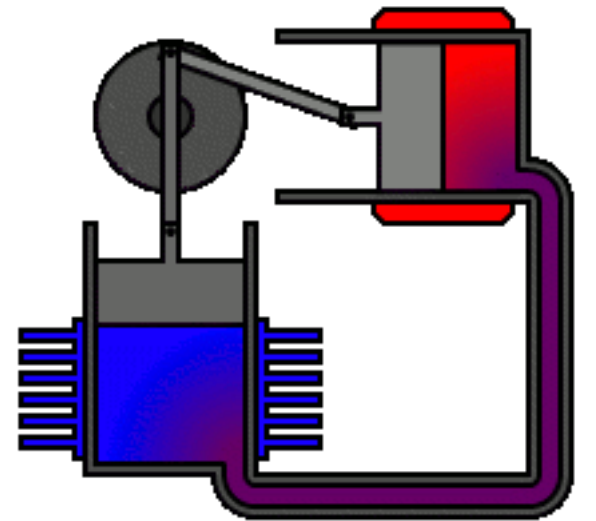
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Stochastic thermodynamics

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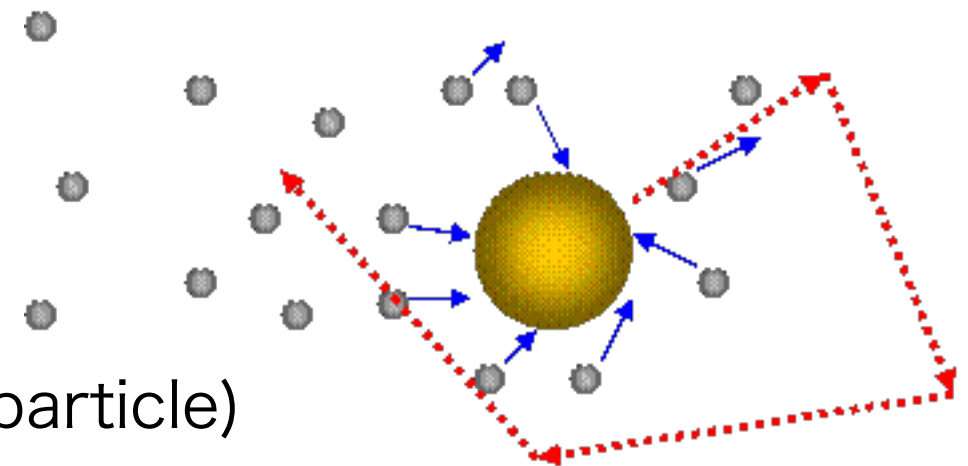
Sekimoto, K. (2010). *Stochastic energetics* (Vol. 799). Springer.

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Information transmission between two systems plays a crucial role!

Introduction

Information thermodynamics

Review

Parrondo, J. M., Horowitz, J. M., & Sagawa, T. (2015). Thermodynamics of information. *Nature physics*, 11(2), 131.

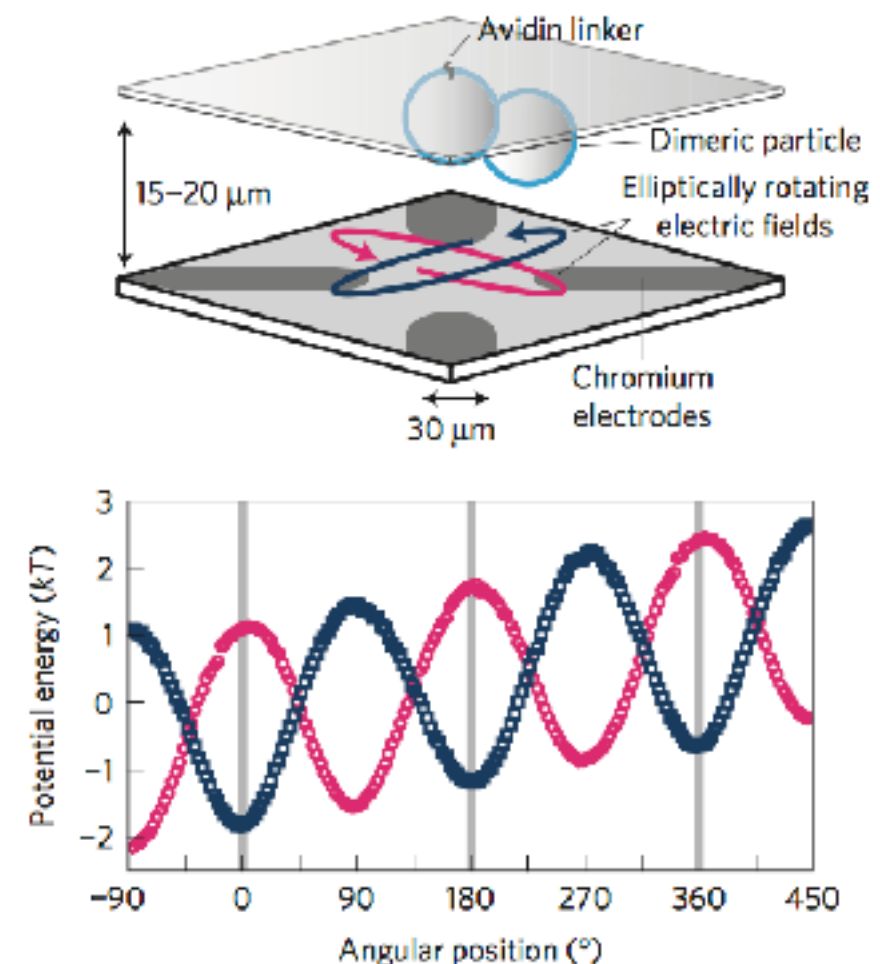
My Ph. D. thesis

Ito, S. (2016). Information thermodynamics on causal networks and its application to biochemical signal transduction. Springer.

We consider the problem of Maxwell's demon
In terms of stochastic thermodynamics.

We can reconsider the theory of
(stochastic) thermodynamics
from the information-theoretic view point.

For example, the second law of thermodynamics
can be generalized for information processing.
(The 2nd law of “information” thermodynamics)



Experimental demonstration of Maxwell's demon

Toyabe, S., Sagawa, T., Ueda, M., Muneyuki, E., & Sano, M. (2010). *Nature physics*, 6(12), 988.

Introduction

Our contributions in the field of information thermodynamics

We derived the second law of information thermodynamics for complex interacting systems. (e.g., 2D Langevin eqs., Master equation, Bayesian networks)

Ito, S., & Sagawa, T. (2013). *Physical review letters*, 111(18), 180603.

Shiraishi, N., Ito, S., Kawaguchi, K., & Sagawa, T. (2015). *New Journal of Physics*, 17(4), 045012.

Ito, S. (2016). *Scientific reports*, 6.

We applied information thermodynamics to biochemical information processing (e.g., sensory adaptation in *E. coli*).

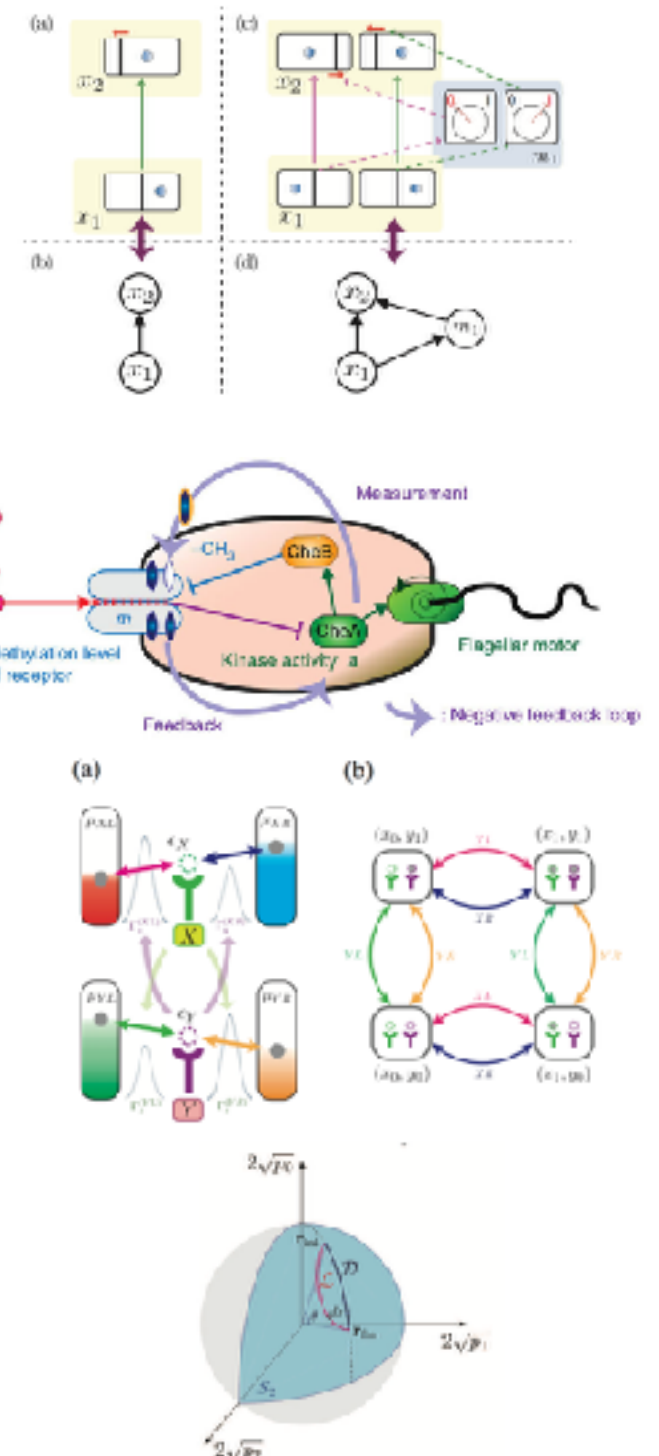
Ito, S., & Sagawa, T. (2015). *Nature communications*, 6.

We obtained the Onsager reciprocal relationship between information flow and thermodynamic flow.

Yamamoto, S., Ito, S., Shiraishi, N., & Sagawa, T. (2016). *Physical Review E*, 94(5), 052121.

We revealed stochastic thermodynamic interpretation of information geometry.

Ito, S. (2017). *arXiv preprint arXiv:1712.04311*.



Introduction

Today's goal

We introduce basics of stochastic thermodynamics for the Langevin equation.

- 1st law of thermodynamics, 2nd law of thermodynamics

We introduce informational quantities.

- mutual information, relative entropy

We derive the second law of information thermodynamics for Langevin equation.

We discuss stochastic thermodynamics in 2D Langevin equations, and clarify the idea of information thermodynamics.

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- Stochastic thermodynamics
- Information theory (Review)
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Thermodynamics (Review)

1st law of thermodynamics

$$dQ = dU - dW \qquad dW = \partial_\lambda U \cdot d\lambda$$

The heat dQ from the thermal bath to the system is given by the difference between the potential energy change of the system dU and the work dW done by the control parameter λ .

2nd law of thermodynamics

$$dS \geq \frac{dQ}{T}$$

The entropy change of the system dS is bounded by the heat dQ per the temperature of the thermal bath T .

Thermodynamics (Review)

2nd law of thermodynamics (Non-negativity)

$$dS \geq \frac{dQ}{T}$$

If dynamics of the system are reversible, the equality holds.
The thermal bath is in equilibrium, the dynamics of heat bath is reversible. We then define the entropy change of the thermal bath as

$$dS_{\text{bath}} = -\frac{dQ}{T}$$

The 2nd law of thermodynamics is given by

$$dS + dS_{\text{bath}} \geq 0$$

(Non-negativity of the total entropy change)

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Stochastic thermodynamics

Langevin equation

$$m_X \ddot{x}(t) = -\gamma_X \dot{x}(t) - \partial_x U_X(x(t), \lambda_X(t)) + \sqrt{2\gamma_X T_X} \xi_X(t)$$

Stochastic differential equation.

White Gaussian noise: ξ_X (Mean 0, variance 1)

Position $x(t)$ at time t , Mass: m_X , Friction coefficient: γ_X . Potential energy: U_X ,

Control parameter: λ_X , Temperature of thermal bath: T_X

Overdamped limit

If relaxation time m_X/γ_X is small enough (compared to the time scale which we consider), we can assume the following overdamped limit. (We here assume $\gamma_X=1$.)

$$\dot{x}(t) = -\partial_x U_X(x(t), \lambda_X(t)) + \sqrt{2T_X} \xi_X(t)$$

Stochastic thermodynamics

1st law of thermodynamics (stochastic thermodynamics)

We consider the following chain rule for the potential energy change dU_X .

$$dU_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) = \dot{x}(t) \circ \partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t))dt + \dot{\lambda}_{\mathcal{X}}(t) \circ \partial_{\lambda_{\mathcal{X}}} U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t))dt$$

where dt is infinitesimal time, \circ is defined as the Stratonovich integral that holds the ordinary calculus (e.g., the chain rule).

Here, we define the work dW_X done by the control parameter, and the heat dQ_X from the thermal bath as follows.

$$dW_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) = \dot{\lambda}_{\mathcal{X}}(t) \circ \partial_{\lambda_{\mathcal{X}}} U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t))dt$$

$$dQ_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) = \dot{x}(t) \circ \partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t))dt$$

We obtain the 1st law of thermodynamics.

$$dQ_{\mathcal{X}} = dU_{\mathcal{X}} - dW_{\mathcal{X}}$$

Stochastic thermodynamics

Definition of the heat

In stochastic thermodynamics, the heat is defined as

$$dQ_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) = \dot{x}(t) \circ \partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) dt$$

By using the Langevin equation

$$\dot{x}(t) = -\partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) + \sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t)$$

we obtain the following expression of the heat

$$dQ_{\mathcal{X}} = \dot{x}(t) \circ (\sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t) - \dot{x}(t)) dt$$

The heat flux $j_{\mathcal{X}} = dQ_{\mathcal{X}}/dt$ is also given by

$$j_{\mathcal{X}}(t) = \dot{x}(t) \circ (\sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t) - \dot{x}(t))$$

This quantity is stochastic, and can be negative.

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Information theory (Review)

Shannon entropy (differential entropy)

Random variable: X . Stochastic value (event): x .

Probability distribution: $p_X(x)$

We define the Shannon entropy (differential entropy) of X as

$$H(X) = - \int dx p_X(x) \ln p_X(x) = \langle -\ln p_X(x) \rangle$$

$\langle \rangle$ is the ensemble average.

By using the joint distribution $p_{X_1, \dots, X_n}(x_1, \dots, x_n)$,
the (joint) Shannon entropy is also defined as

$$\begin{aligned} H(X_1, \dots, X_n) &= - \int dx_1 \cdots dx_n p_{X_1, \dots, X_n}(x_1, \dots, x_n) \ln p_{X_1, \dots, X_n}(x_1, \dots, x_n) \\ &= \langle -\ln p_{X_1, \dots, X_n}(x_1, \dots, x_n) \rangle \end{aligned}$$

Information theory (Review)

Conditional Shannon entropy

In the condition that the random variable Y is known, the conditional Shannon entropy of X is defined as

$$H(X|Y) = H(X, Y) - H(Y)$$

Mutual information

To quantify stochastic correlation between two random variables (X, Y) we define the mutual information as

$$I(X; Y) = H(X) - H(X|Y)$$

In the condition that the random variable Z is known, conditional mutual information between X and Y is defined as

$$I(X; Y|Z) = H(X|Z) - H(X|Y, Z)$$

Information theory (Review)

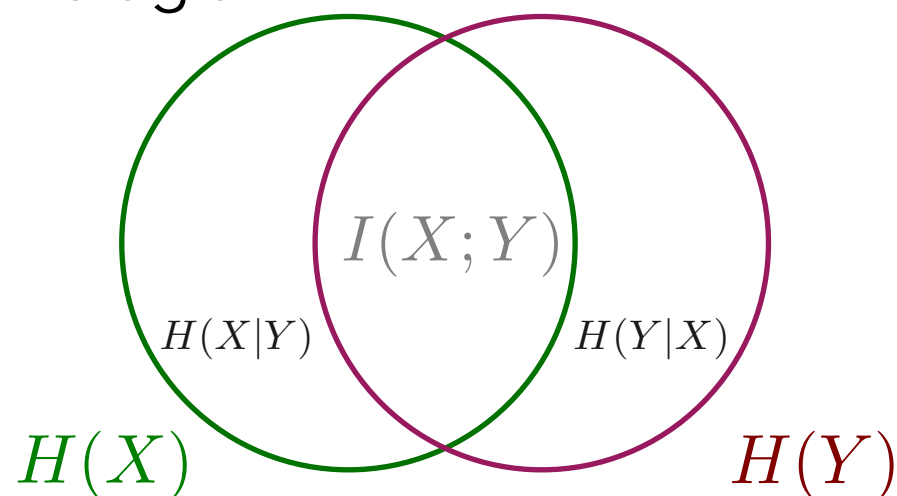
Mathematical properties of mutual information

- Symmetricity $I(X; Y) = I(Y; X)$
- Non-negativity $I(X; Y) \geq 0$

$$I(X; Y) = 0 \quad \text{iff} \quad p_{X,Y}(x, y) = p_X(x)p_Y(y) \quad \text{for any } x, y$$

If X and Y are stochastically independent, it gives 0. (Correlation)

Venn diagram



$$\begin{aligned} I(X; Y) &= H(X) + H(Y) - H(X, Y) \\ &= H(X) - H(X|Y) \\ &= H(Y) - H(Y|X) \end{aligned}$$

Information theory (Review)

Relative entropy (Kullback-Leibler divergence)

As a generalization of mutual information,

We define relative entropy between two distributions $p_X(x)$, $q_X(x)$ as

$$D(p_X || q_X) = \int dx p_X(x) \ln \frac{p_X(x)}{q_X(x)}$$

Mutual information is given by the following relative entropy

$$I(X; Y) = D(p_{X,Y} || p_X p_Y)$$

Information theory (Review)

Non-negativity of the relative entropy

Non-negativity

$$D(p_X || q_X) \geq 0$$

$$D(p_X || q_X) = 0 \quad \text{iff} \quad p_X(x) = q_X(x) \quad \text{for any } x$$

Proof. (abstract)

We use Jensen's inequality.

Convex function: F , Function of x : $G(x)$, Probability distribution $p_X(x)$

$$\int F(G(x))p_X(x)dx \leq F\left(\int G(x)p_X(x)dx\right) \quad \text{or} \quad \langle F(G(x)) \rangle \leq F(\langle G(x) \rangle)$$

If we consider $F=\ln$ and $G(x)=q_X(x)/p_X(x)$, we obtain

$$-D(p_X || q_X) = \langle \ln[q_X(x)/p_X(x)] \rangle \leq \ln[\langle q_X(x)/p_X(x) \rangle] = \ln 1 = 0$$

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2nd law of thermodynamics in stochastic thermodynamics

Transition probability for Langevin equation (Onsager-Machlup)

$$\dot{x}(t) = -\partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(t)) + \sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t)$$

$$\xi_{\mathcal{X}}(t)dt = dB_{\mathcal{X}_t}$$

$$x_t = x(t)$$

$$\lambda_{\mathcal{X}_t} = \lambda_X(t)$$

We consider the following discretization.

$$x_{t+dt} - x_t = -\partial_x U_{\mathcal{X}}(x_t, \lambda_{\mathcal{X}_t})dt + \sqrt{2T_{\mathcal{X}}} dB_{\mathcal{X}_t}$$

Probability of $dB_{\mathcal{X}_t}$ is given by Gaussian.

Jacobian.

$$p(dB_{\mathcal{X}_t}) = \frac{1}{\sqrt{2\pi dt}} \exp \left[-\frac{(dB_{\mathcal{X}_t})^2}{2dt} \right]$$

$$\frac{\partial [dB_{\mathcal{X}_t}]}{\partial x_{t+dt}} = \frac{1}{\sqrt{2T_{\mathcal{X}}}}$$

The transition probability from x_t to x_{t+dt} is given by

$$\mathcal{T}(x_{t+dt}; x_t) = p_{X_{t+dt}|X_t} = \frac{1}{\sqrt{4\pi T_X dt}} \exp \left[-\frac{(x_{t+dt} - x_t + \partial_x U_{\mathcal{X}}(x_t, \lambda_{X_t})dt)^2}{4T_X dt} \right]$$

2nd law of thermodynamics in stochastic thermodynamics

Detailed fluctuation theorem

We consider the backward probability from x_{t+dt} to x_t .

$$p_{B X_t | X_{t+dt}}(x_t | x_{t+dt}) = \mathcal{T}(x_t; x_{t+dt})$$

The ratio between two probabilities gives the heat.

$$\frac{p_{X_{t+dt} | X_t}(x_{t+dt} | x_t)}{p_{B X_t | X_{t+dt}}(x_t | x_{t+dt})} = \exp \left[-\frac{j_{\mathcal{X}}(t)}{T_{\mathcal{X}}} dt \right]$$

(Detailed fluctuation theorem)

$$\mathcal{T}(x_{t+dt}; x_t) = p_{X_{t+dt} | X_t} = \frac{1}{\sqrt{4\pi T_X dt}} \exp \left[-\frac{(x_{t+dt} - x_t + \partial_x U_{\mathcal{X}}(x_t, \lambda_{X_t}) dt)^2}{4T_X dt} \right]$$

$$j_{\mathcal{X}}(t) = \dot{x}(t) \circ (\sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t) - \dot{x}(t))$$

2nd law of thermodynamics in stochastic thermodynamics

2nd law of thermodynamics

We consider the following relative entropy.

$$D(p_{X_{t+dt}|X_t} p_{X_t} || p_{B|X_t|X_{t+dt}} p_{X_{t+dt}}) \geq 0$$

We here use the detailed fluctuation theorem.

$$D(p_{X_{t+dt}|X_t} p_{X_t} || p_{B|X_t|X_{t+dt}} p_{X_{t+dt}}) = -\frac{\langle j_X(t) \rangle dt}{T_X} + H(X_{t+dt}) - H(X_t)$$

The entropy change of X : $dS_X(t) = H(X_{t+dt}) - H(X_t)$

The entropy change of the thermal bath: $dS_{\text{bath}}(t) = -\frac{\langle j_X(t) \rangle}{T_X} dt$

We then obtain the 2nd law of thermodynamics

$$dS_X(t) + dS_{\text{bath}}(t) \geq 0$$

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Information thermodynamics

Langevin equation with memory

The control parameter λ_X depends on the memory state m .

$$\dot{x}(t) = -\partial_x U_{\mathcal{X}}(x(t), \lambda_{\mathcal{X}}(m, t)) + \sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t)$$

Transition probability

The transition probability also depends on the memory state m .

$$\mathcal{T}_m(x_t; x_{t+dt}) = p_{X_{t+dt}|X_t, M}(x_{t+dt}|x_t, m)$$

Information thermodynamics

Detailed fluctuation theorem with memory

For fixed memory state m , we define the backward probability as

$$p_{B X_t | X_{t+dt}, M}(x_t | x_{t+dt}, m) = \mathcal{T}_m(x_t; x_{t+dt})$$

We obtain the detailed fluctuation theorem

$$\frac{p_{X_{t+dt} | X_t, M}(x_{t+dt} | x_t, m)}{p_{B X_t | X_{t+dt}, M}(x_t | x_{t+dt}, m)} = \exp \left[-\frac{j_{\mathcal{X}}(t)}{T_{\mathcal{X}}} dt \right]$$

$$j_{\mathcal{X}}(t) = \dot{x}(t) \circ (\sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t) - \dot{x}(t))$$

Information thermodynamics

2nd law of information thermodynamics

We consider the following relative entropy.

$$D(p_{X_{t+dt}|X_t,M} p_{X_t,M} || p_{B_{X_t}|X_{t+dt},M} p_{X_{t+dt},M}) \geq 0$$

We here use the detailed fluctuation theorem.

$$D(p_{X_{t+dt}|X_t,M} p_{X_t,M} || p_{B_{X_t}|X_{t+dt},M} p_{X_{t+dt},M}) = -\frac{\langle j_X(t) \rangle}{T_X} dt + H(X_{t+dt}, M) - H(X_t, M)$$

The entropy change of X :
$$dS_X(t) = H(X_{t+dt}) - H(X_t)$$

The entropy change of the thermal bath:
$$dS_{\text{bath}}(t) = -\frac{\langle j_X(t) \rangle}{T_X} dt$$

We obtain the 2nd law of information thermodynamics.

$$dS_X(t) + dS_{\text{bath}}(t) \geq I(X_{t+dt}; M) - I(X_t; M)$$

Due to the memory state, we need the term of mutual information.

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Stochastic thermodynamics for 2D Langevin equations

2D Langevin equations

We consider the following 2D Langevin equations.

$$\dot{x}(t) = -\partial_x U_{\mathcal{X}}(x(t), y(t)) + \sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t)$$

$$\dot{y}(t) = -\partial_y U_{\mathcal{Y}}(x(t), y(t)) + \sqrt{2T_{\mathcal{Y}}} \xi_{\mathcal{Y}}(t)$$

White Gaussian noise (mean 0, variance 1, independent): ξ_X, ξ_Y .

Detailed fluctuation theorem

For the following two transition probabilities

$$p_{X_{t+dt}|X_t, Y_t}(x_{t+dt}|x_t, y_t) = \mathcal{T}_{y_t}^{\mathcal{X}}(x_{t+dt}; x_t) \quad p_{Y_{t+dt}|X_t, Y_t}(y_{t+dt}|x_t, y_t) = \mathcal{T}_{x_t}^{\mathcal{Y}}(y_{t+dt}; y_t)$$

we have

$$\frac{\mathcal{T}_{y_t}^{\mathcal{X}}(x_{t+dt}; x_t)}{\mathcal{T}_{y_t}^{\mathcal{X}}(x_t; x_{t+dt})} = \exp \left[-\frac{j_{\mathcal{X}}(t) dt}{T_{\mathcal{X}}} \right] \quad \frac{\mathcal{T}_{x_t}^{\mathcal{Y}}(y_{t+dt}; y_t)}{\mathcal{T}_{x_t}^{\mathcal{Y}}(y_t; y_{t+dt})} = \exp \left[-\frac{j_{\mathcal{Y}}(t) dt}{T_{\mathcal{Y}}} \right]$$

$$\text{where} \quad j_{\mathcal{X}}(t) = \dot{x}(t) \circ (\sqrt{2T_{\mathcal{X}}} \xi_{\mathcal{X}}(t) - \dot{x}(t)) \quad j_{\mathcal{Y}}(t) = \dot{y}(t) \circ (\sqrt{2T_{\mathcal{Y}}} \xi_{\mathcal{Y}}(t) - \dot{y}(t))$$

Stochastic thermodynamics for 2D Langevin equations

2nd law of thermodynamics

We consider the following relative entropy.

$$D(p_{X_{t+dt}|X_t,Y_t} p_{Y_{t+dt}|X_t,Y_t} p_{X_t,Y_t} || p_{B X_t|X_{t+dt},Y_{t+dt}} p_{B Y_t|X_{t+dt},Y_{t+dt}} p_{X_{t+dt},Y_{t+dt}}) \geq 0$$

We here use the detailed fluctuation theorem.

$$\begin{aligned} D(p_{X_{t+dt}|X_t,Y_t} p_{Y_{t+dt}|X_t,Y_t} p_{X_t,Y_t} || p_{B X_t|X_{t+dt},Y_{t+dt}} p_{B Y_t|X_{t+dt},Y_{t+dt}} p_{X_{t+dt},Y_{t+dt}}) \\ = -\frac{\langle j_X(t) \rangle dt}{T_X} - \frac{\langle j_Y(t) \rangle dt}{T_Y} + H(X_{t+dt}, Y_{t+dt}) - H(X_t, Y_t) \end{aligned}$$

The entropy change of X and Y : $dS_{X,Y} = H(X_{t+dt}, Y_{t+dt}) - H(X_t, Y_t)$

The entropy change of the thermal bath:

$$dS_{\text{bath},X} = -\frac{\langle j_X(t) \rangle dt}{T_X}$$

$$dS_{\text{bath},Y} = -\frac{\langle j_Y(t) \rangle dt}{T_Y}$$

We then obtain the 2nd law of thermodynamics

$$dS_{X,Y} + dS_{\text{bath},X} + dS_{\text{bath},Y} \geq 0$$

Stochastic thermodynamics for 2D Langevin equations

2nd law of information thermodynamics

We consider the following relative entropy.

$$D(p_{X_{t+dt}|X_t,Y_t} p_{X_t,Y_t,Y_{t+dt}} || p_{B X_t|X_{t+dt},Y_{t+dt}} p_{Y_t,X_{t+dt},Y_{t+dt}}) \geq 0$$

We here use the detailed fluctuation theorem.

$$\begin{aligned} & D(p_{X_{t+dt}|X_t,Y_t} p_{X_t,Y_t,Y_{t+dt}} || p_{B X_t|X_{t+dt},Y_{t+dt}} p_{Y_t,X_{t+dt},Y_{t+dt}}) \\ &= -\frac{\langle j_{\mathcal{X}}(t) \rangle dt}{T_{\mathcal{X}}} + H(X_{t+dt}) - H(X_t) + I(X_t; \{Y_t, Y_{t+dt}\}) - I(X_{t+dt}; \{Y_t, Y_{t+dt}\}) \end{aligned}$$

The entropy change of X :
$$dS_{\mathcal{X}}(t) = H(X_{t+dt}) - H(X_t)$$

The entropy change of the thermal bath by X :
$$dS_{\text{bath},\mathcal{X}} = -\frac{\langle j_{\mathcal{X}}(t) \rangle dt}{T_{\mathcal{X}}}$$

We then obtain the 2nd law of information thermodynamics

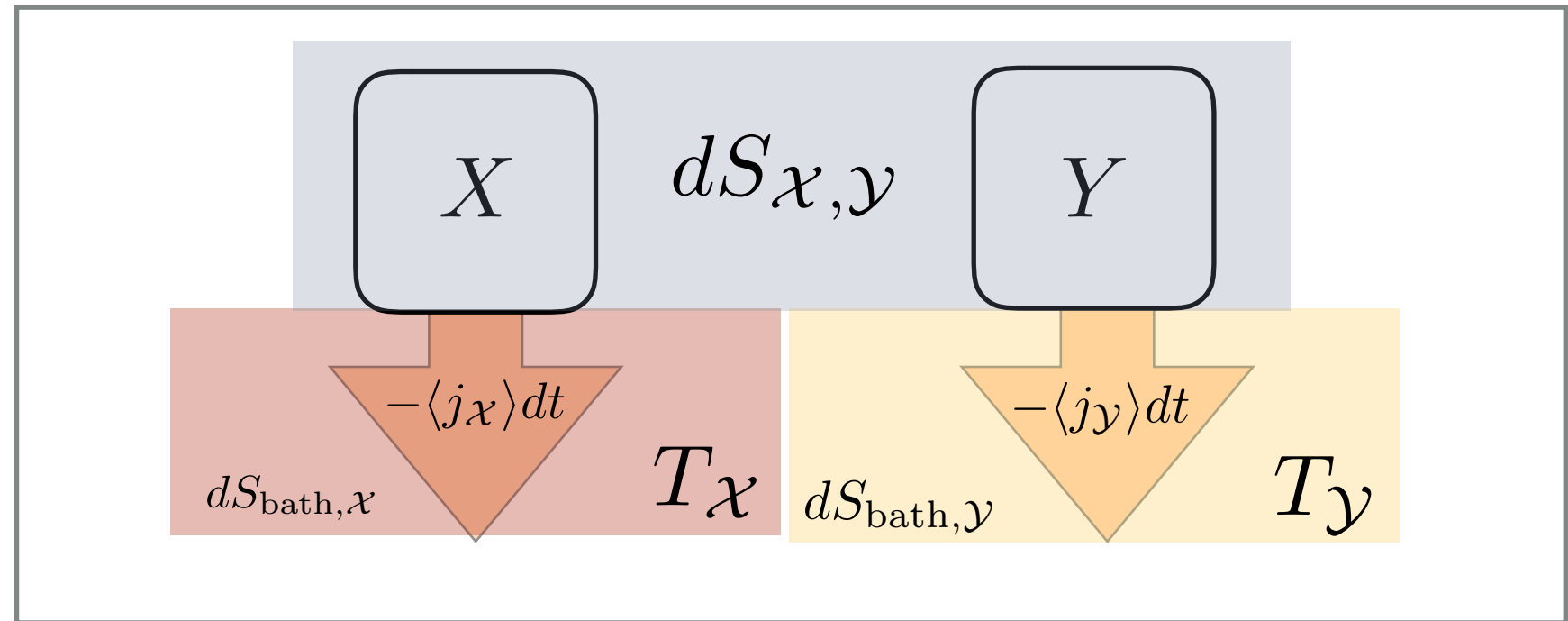
$$dS_{\mathcal{X}} + dS_{\text{bath},\mathcal{X}} \geq I(X_{t+dt}; \{Y_t, Y_{t+dt}\}) - I(X_t; \{Y_t, Y_{t+dt}\}) = dI$$

Stochastic thermodynamics for 2D Langevin equations

Comparison

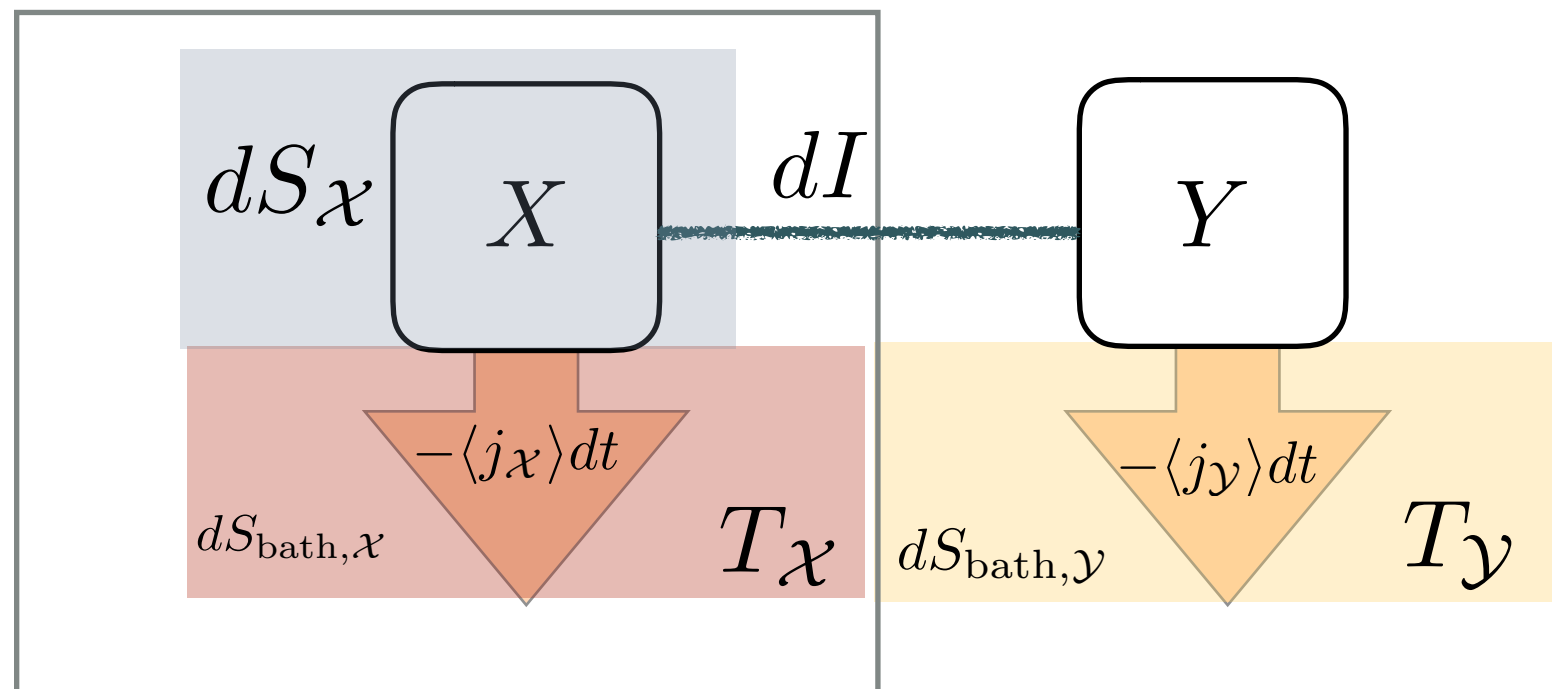
The 2nd law of thermo.

$$dS_{\mathcal{X},\mathcal{Y}} + dS_{\text{bath},\mathcal{X}} + dS_{\text{bath},\mathcal{Y}} \geq 0$$



The 2nd law of info. thermo.

$$dS_{\mathcal{X}} + dS_{\text{bath},\mathcal{X}} \geq dI$$



Summary

For Langevin equation, the 1st law is given by the chain rule, and the 2nd law is given by non-negativity of the relative entropy.

If there is a memory state, the 2nd law is modified because we have to consider the relative entropy with a memory state.

The modified term is given by mutual information difference.

If we consider 2D Langevin equations, we have two choices of the relative entropy. One gives the 2nd law of thermodynamics, and another gives the 2nd law of information thermodynamics.

The 2nd law of information thermodynamics can be considered as the 2nd law for a subsystem.