Thermodynamics of information geometry and a generalization of the Glansdorff-Prigogine criterion for stability

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5th East Asia Joint Seminars on Statistical Physics,
Beijing, Oct. 23.

Related papers:

Sosuke Ito, Phys. Rev. Lett. **121**, 030605 (2018), Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018).
Sosuke Ito, arXiv, 1908.09446 (2019).

Table of contents

- **Background (Geometry of thermodynamics)**

- **Thermodynamics of information geometry**

- **A generalization of the Glansdorff-Prigogine criterion for stability**

Motivation

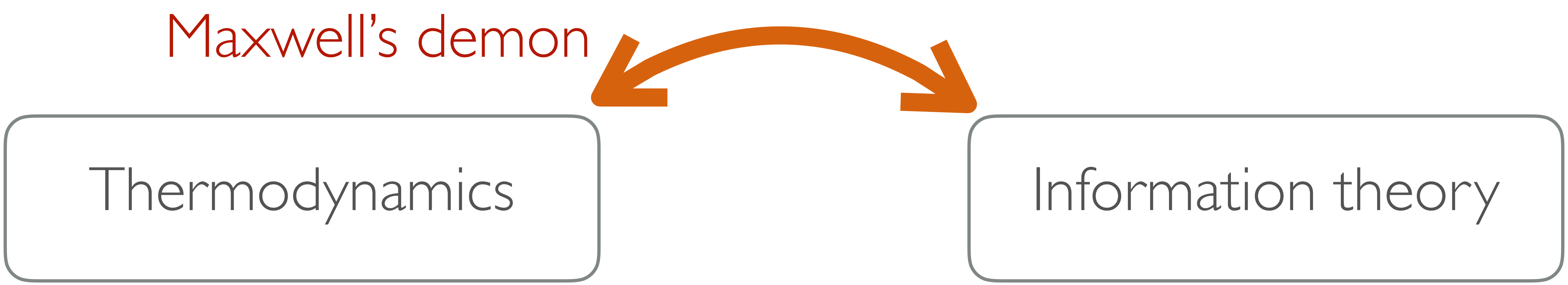
- **A unified theory of thermodynamics and information**

Our contributions:

Ito, S., & Sagawa, T. (2013). Information thermodynamics on causal networks. *Physical review letters*, *111*(18), 180603.

Ito, S., & Sagawa, T. (2015). Maxwell's demon in biochemical signal transduction with feedback loop. *Nature communications*, *6*, 7498.

…etc.



Motivation

- **A unified theory of thermodynamics and information**

Thermodynamics

Information theory

Information geometry (1943-)
Ruppeiner geometry(1979)
Thermodynamic length (2007)

Differential geometry

Ruppeiner, G. (1979). Thermodynamics: A Riemannian geometric model. *Physical Review A*, *20*(4), 1608.
Crooks, G. E. (2007). Measuring thermodynamic length. *Physical Review Letters*, *99*(10), 100602.
Amari, S. I. (2016). *Information geometry and its applications*. Springer Japan.

Background

- **Differential geometry of thermodynamics**
  - Ruppeiner geometry (1979)

$$g^{\mathrm{R}}_{ij} = -\partial_{\theta_i}\partial_{\theta_j} S$$

S : Entropy (Thermodynamics)

Differential geometry

$$ds^2 = \sum_{i,j} g_{ij} d\theta_i d\theta_j$$

ds : Line element

g_{ij} : Metric

θ_i : i-th parameter of thermodynamics

Ruppeiner, G. (1979). Thermodynamics: A Riemannian geometric model. *Physical Review A*, *20*(4), 1608.

Background

- **Differential geometry of thermodynamics**
  - Ruppeiner geometry (1979)

$$g^{\mathrm{R}}_{ij} = -\partial_{\theta_i}\partial_{\theta_j} S$$

S : Entropy (Thermodynamics)

  - Thermodynamic length (2007)

$$g^{\mathrm{F}}_{ij} = -\mathbb{E}[\partial_{\theta_i}\partial_{\theta_j} \ln p_{\mathrm{can}}]$$

p_{can} : Gibbs ensemble (Statistical physics) $\mathbb{E}$: Expected value

Differential geometry

$$ds^2 = \sum_{i,j} g_{ij} d\theta_i d\theta_j$$

ds : Line element

g_{ij} : Metric

θ_i : i-th parameter of thermodynamics

Ruppeiner, G. (1979). Thermodynamics: A Riemannian geometric model. *Physical Review A*, *20*(4), 1608.

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Information geometry

- **Differential geometry of probability**

$$ds^2 = \sum_{\mu,\nu} g_{\mu\nu} d\theta_\mu d\theta_\nu \qquad \left(\left(\frac{ds}{dt}\right)^2 = \sum_{\mu,\nu} g_{\mu\nu} \frac{d\theta_\mu}{dt} \frac{d\theta_\nu}{dt} \right)$$

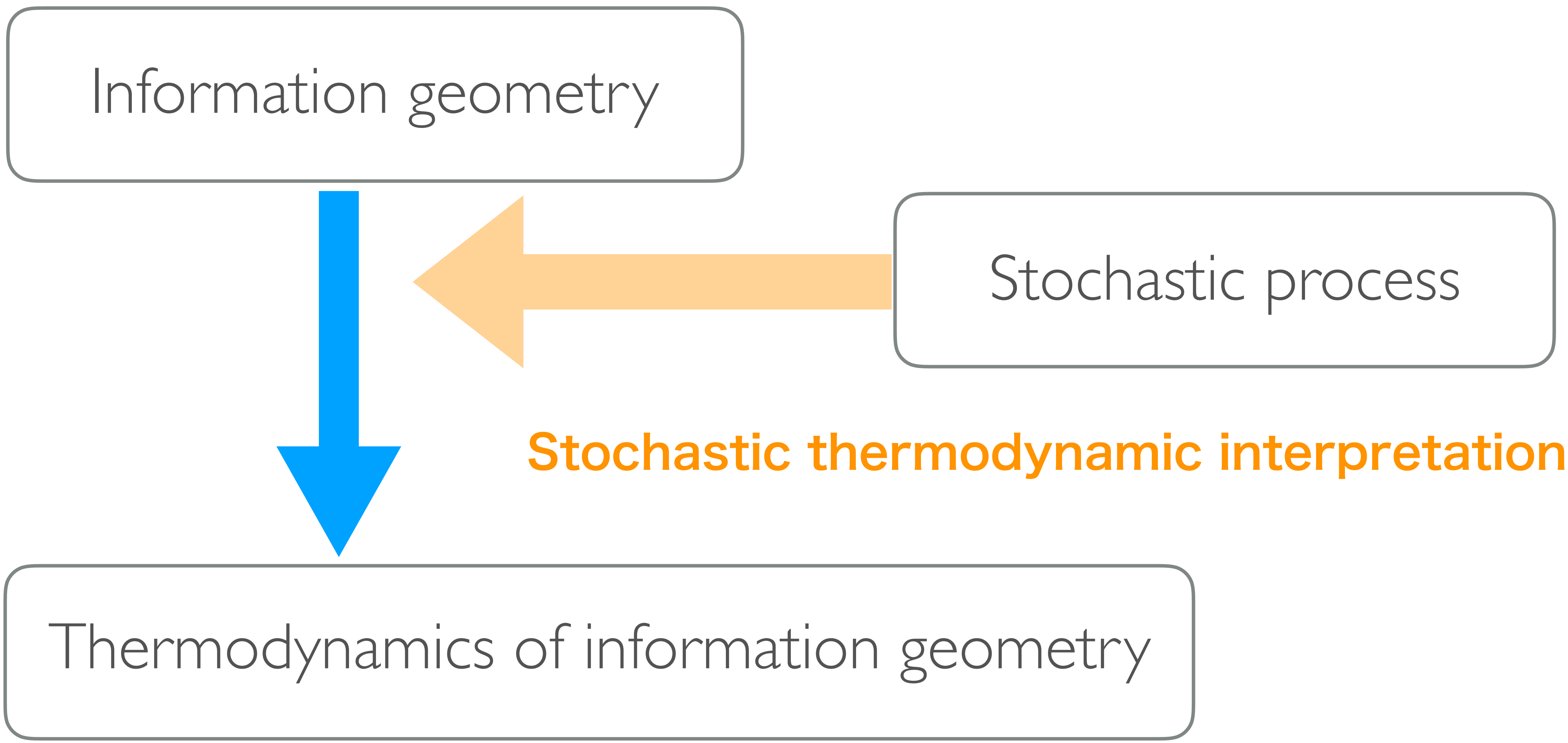
$$g_{\mu\nu} = -\mathbb{E}[\partial_{\theta_\mu} \partial_{\theta_\nu} \ln p]$$: Fisher information matrix

p : probability

θ_μ : **μ**-th parameter of probability

Textbook; Amari, S. I. (2016). *Information geometry and its applications*. Springer Japan.

Thermodynamics of information geometry



<u>Sosuke Ito,</u> Phys. Rev. Lett. **121**, 030605 (2018)

<u>As a generalization of differential geometry of thermodynamics</u>

Thermodynamic interpretations of information geometry

- **Near-equilibrium condition**

Canonical distribution: $p(x,t) = \dfrac{\exp(-\beta U(x,t))}{\sum_x \exp(-\beta U(x,t))}$

$\approx$

$$\left(\frac{ds}{dt}\right)^2 = \beta^2 \left[\mathbb{E}[(\partial_t U)^2] - (\mathbb{E}[\partial_t U])^2\right]$$

Variance of work

Thermodynamic interpretations of information geometry

- **Non-equilibrium condition**

Sosuke Ito, Phys. Rev. Lett. **121**, 030605 (2018).

$$\frac{dp_i}{dt} = \sum_j [W_{ij}p_j - W_{ji}p_i] = \sum_j J_{ij}$$:Master equation

$$\left(\frac{ds}{dt}\right)^2 = \left\langle \frac{d\Delta\sigma^{\mathrm{bath}}}{dt} \right\rangle - \left\langle \frac{dF}{dt} \right\rangle$$

$$\langle A \rangle := \sum_{i,j|i>j} A_{ij} J_{ij}$$

Stochastic entropy production: $F_{ij} = \ln \frac{W_{ij}p_j}{W_{ji}p_i}$

Entropy change of the heat bath: $\Delta\sigma^{\mathrm{bath}}_{ij} = \ln \frac{W_{ij}}{W_{ji}}$

Thermodynamic uncertainty relationships (TURs) from thermodynamics of information geometry

- **Trade-off relationship between (ds/dt)² and other quantities**

Speed limit:
$$\tau \int \left(\frac{ds}{dt}\right)^2 dt \geq \left(\int ds\right)^2$$

Geodesic:
$$\int ds \geq 2\cos^{-1}\left(\sum_i \sqrt{p_i(t=0)}\sqrt{p_i(t=\tau)}\right)$$

As a thermodynamic generalization of the quantum speed limit

Trade-off relationship between thermodynamic cost and speed

Sosuke Ito, Phys. Rev. Lett. **121**, 030605 (2018), Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018).

Thermodynamic uncertainty relationships (TURs) from thermodynamics of information geometry

- **Trade-off relationship between (ds/dt)^2 and other quantities**

Cramér-Rao inequality:
(for any observable R)

$$\frac{\mathrm{var}[R]}{(d\mathbb{E}[R]/dt)^2}\left(\frac{ds}{dt}\right)^2 \geq 1$$

$$\mathrm{var}[R] = \mathbb{E}[R^2] - (\mathbb{E}[R])^2$$

Trade-off relationship between thermodynamic cost and a variance of any observable

Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018).

cf.) Thermodynamic uncertainty

D_{R} : diffusion coefficient of R

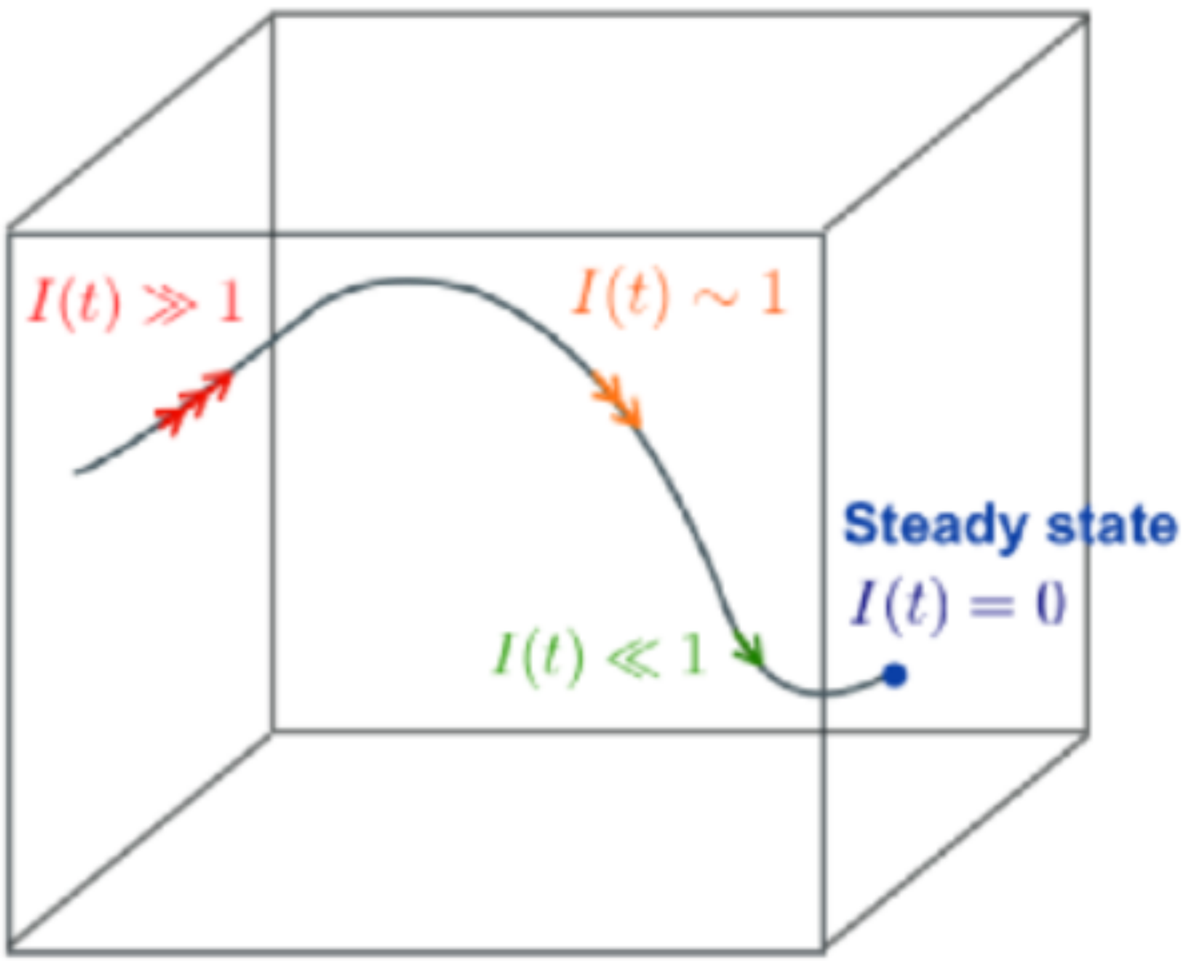
σ_{tot} : entropy production

$$\frac{D_R}{(d\mathbb{E}\left[R\right]/dt)^2}\sigma_{\mathrm{tot}} \geq 1$$

See also [A. Dechant, *Journal of Physics A 52*(3), 035001 (2018).]

Relaxation (Monotonicity)

- **A law of relaxation to the steady state**



Monotonicity

$$d_t I(t) \leq 0$$

$$I(t) = \left(\frac{ds}{dt}\right)^2$$

Relaxation process:

$$\frac{dW_{ij}}{dt} = 0$$

$$\Rightarrow \quad \frac{d}{dt}\left[\left(\frac{ds}{dt}\right)^2\right] \leq 0$$

Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018).

Relaxation (Monotonicity)

Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018). [resubmitted in 2019]

For the Fokker-Planck equation

$$\partial_t p = -\partial_x j$$

$$\nu = \frac{j}{p} = \mu(f - k_{\mathrm{B}} T \partial_x \ln p)$$

A tighter bound

$$\left\langle \frac{\dot{\nu}^2}{\mu} \right\rangle = \frac{1}{k_{\mathrm{B}}T} \langle \dot{f} \dot{\nu} \rangle - \frac{1}{2} \frac{d}{dt} \left[\left(\frac{ds}{dt} \right)^2 \right] \geq 0$$

cf.) the 2nd law of thermodynamics

S_{sys} : Shannon entropy

$$\left\langle \frac{\nu^2}{\mu} \right\rangle = \frac{1}{k_{\mathrm{B}}T} \langle f \nu \rangle + \frac{d}{dt} S_{\mathrm{sys}} \geq 0$$

Table of contents

- **Background (Geometry of thermodynamics)**
- **Thermodynamics of information geometry**
- **A generalization of the Glansdorff-Prigogine criterion for stability**

Glansdorff-Prigogine criterion for stability (1970)

- **Criterion for stability of a steady state**

$\delta^2\sigma$: Excess entropy production
(2nd order difference from
the entropy production in a steady state)

$\delta^2\sigma \geq 0$: this steady state is STABLE

$\delta^2\sigma < 0$: this steady state is UNSTABLE

Glansdorff, P., & Prigogine, I. Non-equilibrium stability theory. Physica, 46, 344-366 (1970).
Glansdorff, P., & Prigogine, I. Thermodynamic theory of structure, stability and fluctuations. (Wiley, 1971)

The excess entropy production in the master equation

Schnakenberg, J. (1976). Network theory of microscopic and macroscopic behavior of master equation systems. *Reviews of Modern physics*, *48*(4), 571.

Master equation: $$\frac{dp_i}{dt} = \sum_j [W_{ij}p_j - W_{ji}p_i] = \sum_j J_{ij}$$

Excess entropy production: $$\delta^2\sigma = \sum_{i,j|i>j} \delta J_{ij}\delta F_{ij}$$

$$J_{ij} = W_{ij}p_j - W_{ji}p_i \qquad F_{ij} = \ln\frac{W_{ij}p_j}{W_{ji}p_i}$$

$$\delta J_{ij} = J_{ij} - J_{ij}|_{\boldsymbol{p}=\bar{\boldsymbol{p}}} \qquad \delta F_{ij} = F_{ij} - F_{ij}|_{\boldsymbol{p}=\bar{\boldsymbol{p}}}$$

cf.) entropy production:

$$\sigma_{\mathrm{tot}} = \sum_{i,j|i>j} F_{ij}J_{ij}$$

Stationary state (fixed point) $\bar{\boldsymbol{p}}$: $\frac{d\bar{p}_i}{dt} = 0$

The Lyapunov function and the Lyapunov stability for the linear master equation

- **For the linear master equation (W does not depend on p)**

$$\delta^2\sigma = -\frac{d}{dt}[\delta^2\mathcal{L}]$$

$$\delta p_i = p_i - \bar{p}_i$$

Lyapunov function:

$$\delta^2\mathcal{L} = \frac{1}{2}\sum_i \frac{(\delta p_i)^2}{\bar{p}_i}$$

The Glansdorff-Prigogine criterion is a Lyapunov stability criterion.

$\frac{d}{dt}\delta^2\mathcal{L} \leq 0$:Lyapunov stable

$\frac{d}{dt}\delta^2\mathcal{L} > 0$:Lyapunov unstable

Lyapunov function

$$\delta^2\mathcal{L} \geq 0,$$

$$\delta^2\mathcal{L} = 0 \quad \text{iff} \quad \boldsymbol{p} = \bar{\boldsymbol{p}}$$

The Lyapunov function and information geometry

- **Around the steady state (the linear master equation)**

Lyapunov function:

$$\delta^2 \mathcal{L} = \frac{1}{2} \sum_i \frac{(\delta p_i)^2}{\bar{p}_i}$$

The line element:
(information geometry)

$$ds^2 = \sum_{\mu,\nu} -\mathbb{E}[\partial_{\theta_\mu} \partial_{\theta_\nu} \ln p] d\theta_\mu d\theta_\nu = \sum_i \frac{(dp_i)^2}{p_i}$$

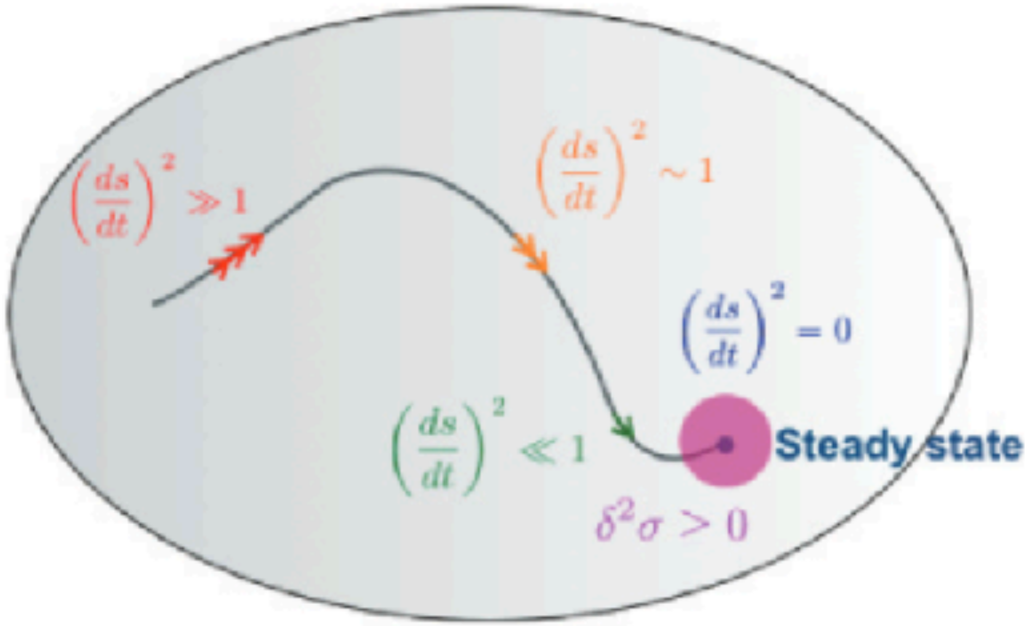
$$\boldsymbol{p} \simeq \bar{\boldsymbol{p}}, \left(\frac{dW_{ij}}{dp_k} = 0 \right) \quad \Rightarrow \quad \delta^2 \sigma \simeq -\frac{1}{2} \frac{d}{dt} [ds^2]$$

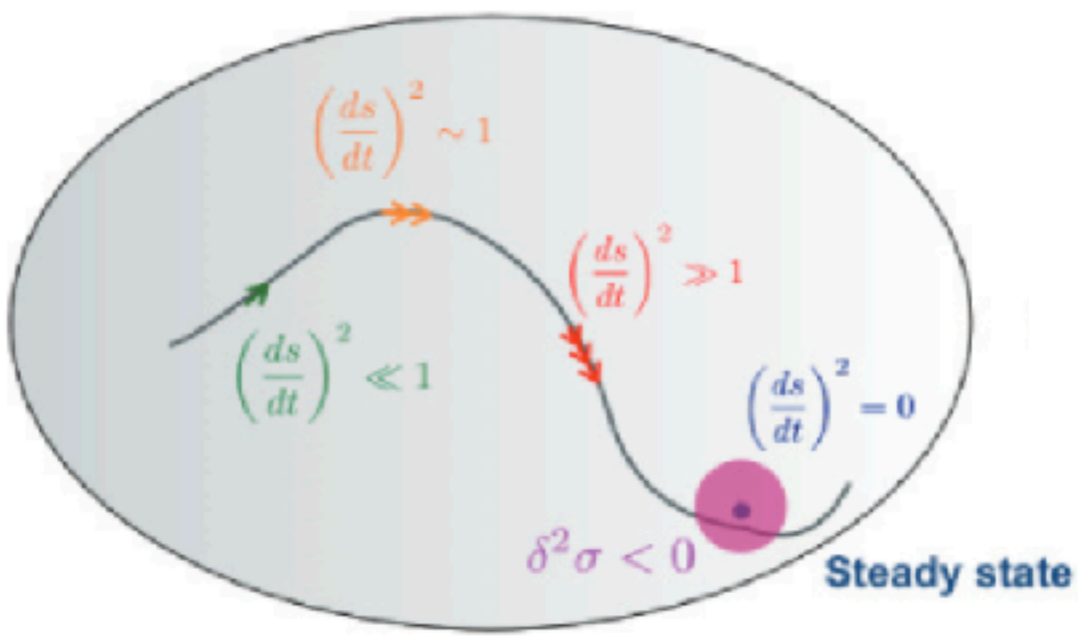
Based on this relationship,
we generalize the Glansdorff-Prigogine criterion.

A generalization of the Glansdorff-Prigogine criterion for stability

Sosuke Ito, arXiv, 1908.09446 (2019).

- **Schematic of our criterion**





Stable:

$$\frac{d}{dt}\left[\left(\frac{ds}{dt}\right)^2\right] \leq 0$$

Unstable:

$$\frac{d}{dt}\left[\left(\frac{ds}{dt}\right)^2\right] > 0$$

Supremacy of our information geometric criterion compared to the Glansdorff-Prigogine criterion

✅ Our criterion does work even for the non-linear master equation

✅ Applicable for any non-stationary dynamics

✅ Based on thermodynamic uncertainty (TURs)

Moreover, our result gives the relationship between the Onsager coefficient $L_{\mu\nu}$ and the Fisher information matrix $g^J_{\mu,\nu}$ around the equilibrium state.

$$\sum_{\mu\nu} L_{\mu\nu}\delta J_\mu \delta J_\nu = -\frac{1}{2}\frac{d}{dt}\left[\sum_{\mu,\nu} g^J_{\mu,\nu}\delta J_\mu \delta J_\nu\right]$$

$L_{\mu\nu}$: Onsager coefficient

$$g^J_{\mu,\nu} = -\mathbb{E}[\partial_{J_\mu}\partial_{J_\nu}\ln p]$$

J_μ : μ-th mode of flow

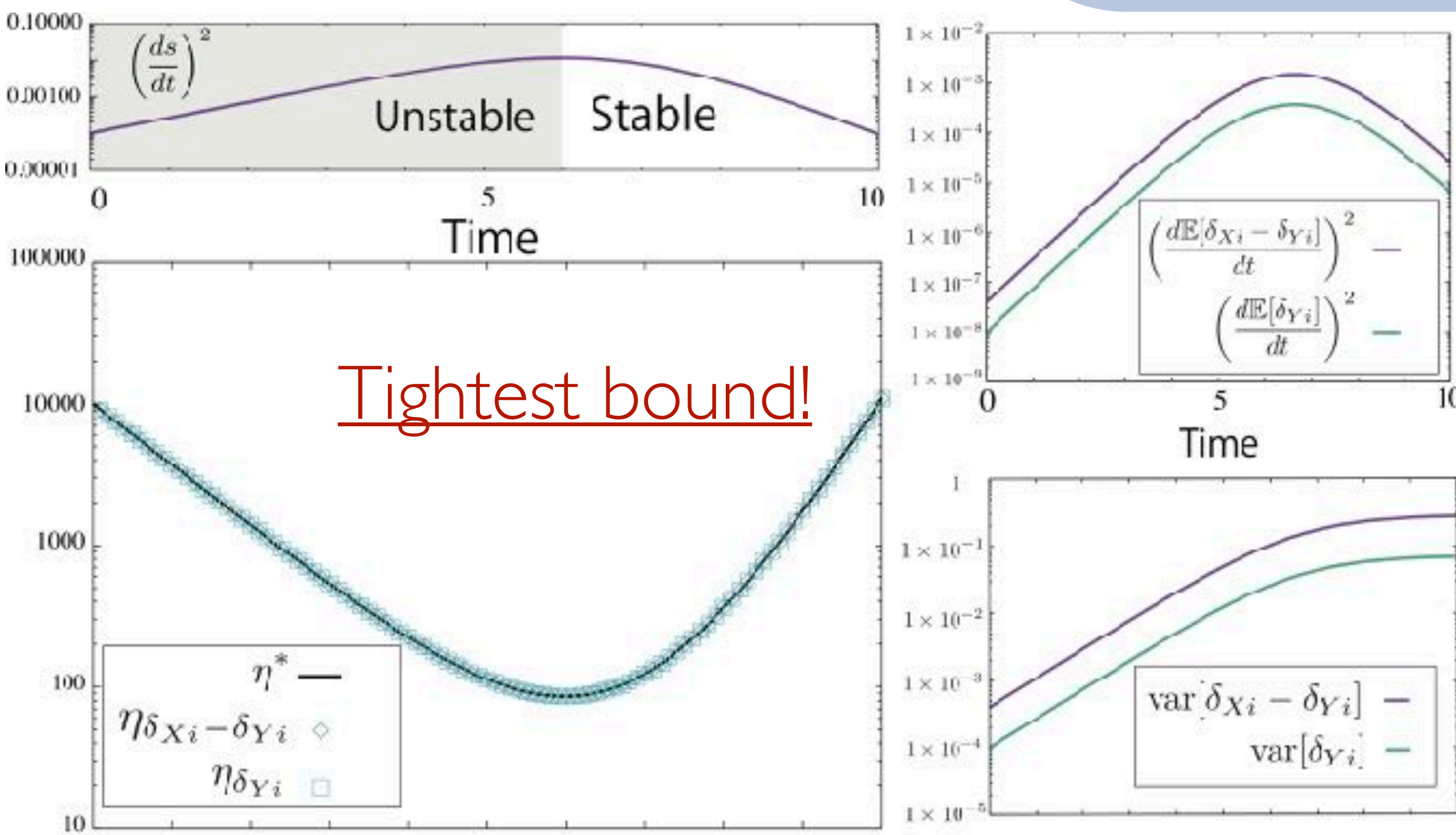
Example : Autocatalytic reaction

Autocatalytic reaction

$$X + Y \rightleftharpoons 2X$$

The Cramér-Rao inequality

$$\eta_R = \frac{\mathrm{var}[R]}{\left(\frac{d\mathbb{E}[R]}{dt}\right)^2} \geq \eta^* = \frac{1}{\left(\frac{ds}{dt}\right)^2}$$

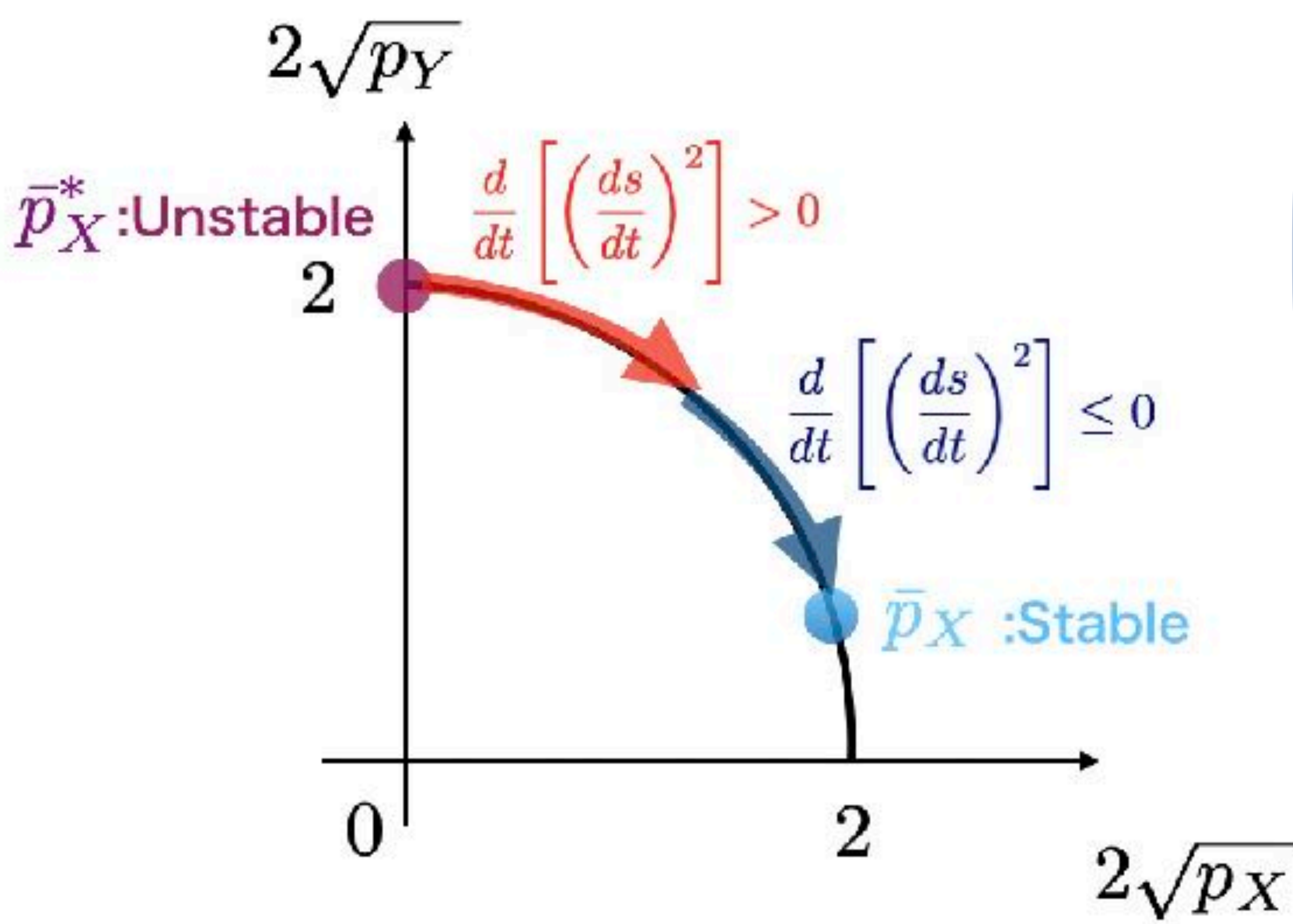


Tightest bound!

We can discuss stability quantitatively based on TURs.

Schematic of our geometric criterion for stability

✅ The speed $(ds/dt)^2$ in information geometry tell us stability of the system.



Information geometry
= Geometry of a circle

$$ds^2 = (d[2\sqrt{p_X}])^2 + (d[2\sqrt{p_Y}])^2$$
$$(\sqrt{p_X})^2 + (\sqrt{p_Y})^2 = 1$$
$$p_X \geq 0, p_Y \geq 0$$

$$X + Y \rightleftharpoons 2X$$

$$p_X = \frac{[X]}{[X]+[Y]} \quad p_Y = \frac{[Y]}{[X]+[Y]}$$

Summary

An information geometric theory of thermodynamics

We found a new thermodynamic interpretation of information geometry.

We obtain several TURs from this framework.

Our framework can be regarded as a generalization of the Glansdorff-Prigogine criterion for stability.

Sosuke Ito, Phys. Rev. Lett. **121**, 030605 (2018), :Thermodynamic interpretation, Speed limit

Sosuke Ito and Andreas Dechant, arXiv:1810.06832 (2018). :TURs, Cramér-Rao, Monotonicity

Sosuke Ito, arXiv, 1908.09446 (2019). :The Glansdorff-Prigogine criterion for stability