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

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

**Information theory**
- 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.
• Differential geometry of thermodynamics

• Ruppeiner geometry (1979)

\[ g^R_{ij} = -\partial_{\theta_i} \partial_{\theta_j} S \]

\( S \): Entropy (Thermodynamics)

Differential geometry

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

\( ds \): Line element

\( g_{ij} \): Metric

\( \theta_i \): 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)
    \[
    g_R^{ij} = -\partial_{\theta_i} \partial_{\theta_j} S
    \]
    \(S\) : Entropy (Thermodynamics)
  - Thermodynamic length (2007)
    \[
    g^F_{ij} = -\mathbb{E}[\partial_{\theta_i} \partial_{\theta_j} \ln p_{\text{can}}]
    \]
    \(p_{\text{can}}\) : Gibbs ensemble (Statistical physics) \(\mathbb{E}\) : Expected value

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

\(ds\) : Line element
\(g_{ij}\) : Metric
\(\theta_i\) : i-th parameter of thermodynamics

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.
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• Background (Geometry of thermodynamics)

• Thermodynamics of information geometry

• A generalization of the Glansdorff-Prigogine criterion for stability
Information geometry

• Differential geometry of probability

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

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

\[ p \text{ : probability} \]
\[ \theta_\mu \text{ : } \mu\text{-th parameter of probability} \]
Thermodynamics of information geometry

Information geometry

Stochastic process

Stochastic thermodynamic interpretation

Thermodynamics of information geometry

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

As a generalization of differential geometry of thermodynamics
Thermodynamic interpretations of information geometry

• Near-equilibrium condition

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

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

Variance of work
Thermodynamic interpretations of information geometry

- **Non-equilibrium condition**

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

: Master equation

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

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

Stochastic entropy production:

\[
F_{ij} = \ln \frac{W_{ij}p_j}{W_{ji}p_i}
\]

Entropy change of the heat bath:

\[
\Delta \sigma_{ij}^{\text{bath}} = \ln \frac{W_{ij}}{W_{ji}}
\]

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

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

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

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

  cf.) Thermodynamic uncertainty

  \(D_R\) : diffusion coefficient of \(R\)

  \(\sigma_{\text{tot}}\) : entropy production

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

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

- A law of relaxation to the steady state

\[ d_t I(t) \leq 0 \]
\[ I(t) = \left( \frac{d s}{d t} \right)^2 \]

Relaxation process:

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

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

For the Fokker-Planck equation

\[ \partial_t \rho = -\partial_x j \]
\[ j = \frac{\dot{\rho}}{\rho} = \mu (f - k_B T \partial_x \ln \rho) \]

A tighter bound

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

cf.) the 2nd law of thermodynamics

\[ S_{sys} : \text{Shannon entropy} \]

\[ \left\langle \frac{\nu^2}{\mu} \right\rangle = \frac{1}{k_B T} \langle f \nu \rangle + \frac{d}{dt} S_{sys} \geq 0 \]
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• Background (Geometry of thermodynamics)

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• A generalization of the Glansdorff-Prigogine criterion for stability
Glansdorff-Prigogine criterion for stability (1970)

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

\[ \delta^2 \sigma \ : \text{Excess entropy production} \]

(2nd order difference from the entropy production in a steady state)

\[ \delta^2 \sigma \geq 0 \ : \text{this steady state is STABLE} \]

\[ \delta^2 \sigma < 0 \ : \text{this steady state is UNSTABLE} \]

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

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

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

\[
J_{ij} = W_{ij} p_j - W_{ji} p_i \quad F_{ij} = \ln \frac{W_{ij} p_j}{W_{ji} p_i}
\]

\[
\delta J_{ij} = J_{ij} - J_{ij} \big|_{p=\bar{p}}
\]

\[
\delta F_{ij} = F_{ij} - F_{ij} \big|_{p=\bar{p}}
\]

Stationary state (fixed point) \[
\bar{p} : \quad \frac{d\bar{p}_i}{dt} = 0
\]

Schnakenberg, J. (1976). Network theory of microscopic and macroscopic behavior of master equation systems. *Reviews of Modern physics*, 48(4), 571.
The Lyapunov function and the Lyapunov stability for the linear master equation

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

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

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.

\[ \frac{d}{dt} \delta^2 \mathcal{L} \leq 0 \quad : \text{Lyapunov stable} \]

\[ \frac{d}{dt} \delta^2 \mathcal{L} > 0 \quad : \text{Lyapunov unstable} \]

Lyapunov function

\[ \delta^2 \mathcal{L} \geq 0, \quad \text{iff} \quad p = \bar{p} \]
The Lyapunov function and information geometry

- Around the steady state (the linear master equation)

Lyapunov function: \[ \delta^2 \mathcal{L} = \frac{1}{2} \sum_i \frac{\left( \delta p_i \right)^2}{\bar{p}_i} \]

The line element: (information geometry)

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

\[ p \simeq \bar{p}, \left( \frac{dW_{ij}}{dp_k} = 0 \right) \]

Based on this relationship, we generalize the Glansdorff-Prigogine criterion.
A generalization of the Glansdorff-Prigogine criterion for stability

• Schematic of our criterion

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

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

Sosuke Ito, arXiv, 1908.09446 (2019).
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 $g_{\mu,\nu}$ around the equilibrium state.

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

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

$g_{\mu,\nu}^J = -\mathbb{E}[\partial J_{\mu} \partial J_{\nu} \ln p]$  

$J_{\mu}$: $\mu$-th mode of flow
Example: Autocatalytic reaction

\[ X + Y \rightleftharpoons 2X \]

The Cramér-Rao inequality

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

We can discuss stability quantitatively based on TURs.
The speed \((ds/dt)^2\) in information geometry tell us stability of the system.

**Information geometry**

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

\[ X + Y \Rightarrow 2X \]

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