Information geometry, several variants of thermodynamic uncertainty relations, and speed limits

The Universal Biology Institute, The University of Tokyo/JST PRESTO
Sosuke Ito

May 28th, 2020
CSH Online Workshop
“Stochastic thermodynamics of complex systems”

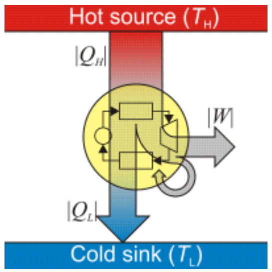
Reference

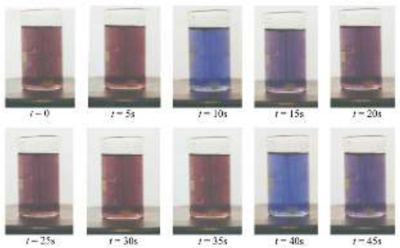
Sosuke Ito, Phys. Rev. Lett. **121**, 030605. (2018).
Sosuke Ito and Andreas Dechant, to appear in Phys. Rev. X (2020). [arXiv 1810.06832 (2018).]
Sosuke Ito, arXiv 1908.09446 (2019).
Kohei Yoshimura and Sosuke Ito, arXiv 2005.08444 (2020).

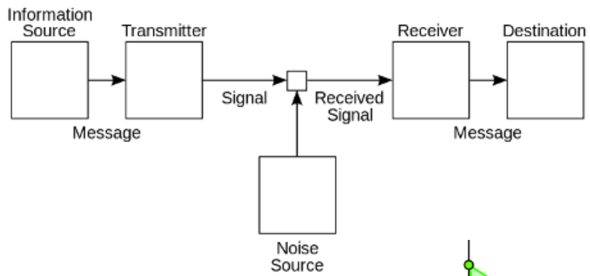
Concept

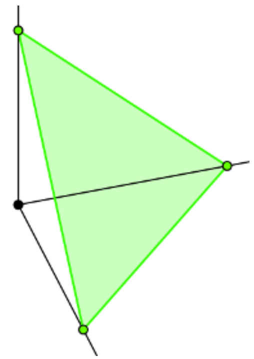
- **A unified theory of thermodynamics and information**

Thermodynamics ⟷ Information theory (Information geometry)









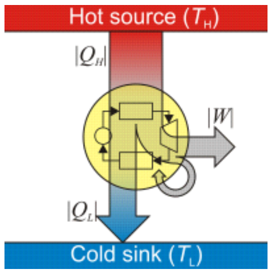
(Pictures from Wikipedia)

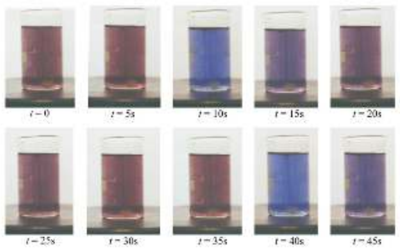
Concept

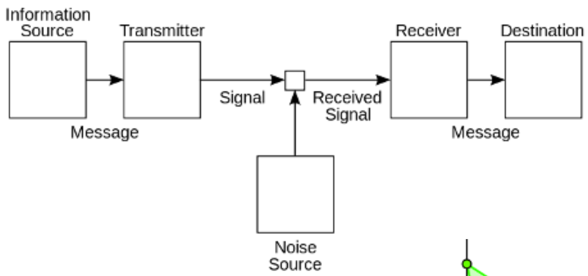
Two key concepts

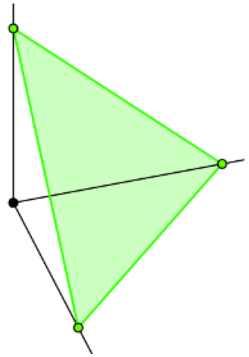
- **A unified t**

Thermodynamics ⟷ Information theory (Information geometry)









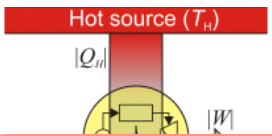
(Pictures from Wikipedia)

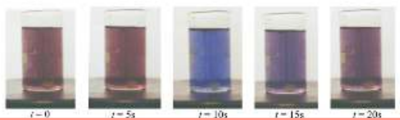
Concept

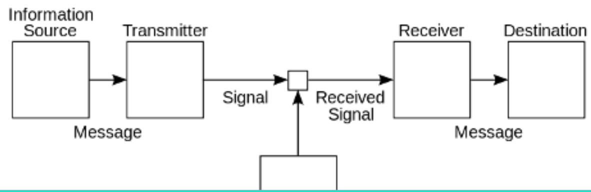
Two key concepts

- **A unified t**

Thermodynamics ⟷ Information theory (Information geometry)







The entropy production

The Fisher information

(Pictures from Wikipedia)

The entropy production

The entropy production σ

A thermodynamic measure of irreversibility

For the Fokker-Planck equation

$$\partial_t P(x;t) = -\partial_x j(x;t)$$

$$j = P(F - T\partial_x \ln P) = \nu P$$

$P(x;t)$: probability of position x at time t
F : force
T : temperature
j : flux
ν : mean local velocity
($k_{\mathrm{B}} = 1$)

$$\sigma = \frac{1}{T}\int dx P\nu^2 = \frac{1}{T}\int dx \frac{j^2}{P}$$

The Fisher information

The Fisher information (of time) ds^2/dt^2

An informational measure of estimation

In information geometry, it gives an information-geometric speed on the probability simplex.

$$\frac{ds^2}{dt^2} = \int dx P (\partial_t \ln P)^2 = \int dx \frac{(\partial_t P)^2}{P}$$

For the Fokker-Planck equation

$$\frac{ds^2}{dt^2} = \int dx \frac{(\partial_x j)^2}{P}$$

cf.) $\sigma = \frac{1}{T} \int dx \frac{j^2}{P}$

Comparison

The entropy production σ

$$\sigma = \frac{1}{T}\int dx \frac{j^2}{P}$$

Nonnegativity:
(The 2nd law)

$$\sigma \geq 0$$

Equilibrium state:

$$\sigma = 0 \Leftrightarrow j = 0$$

Lower bound:
The thermodynamic uncertainty relation

The Fisher information ds^2/dt^2

$$\frac{ds^2}{dt^2} = \int dx \frac{(\partial_t P)^2}{P}$$

Nonnegativity:

$$\frac{ds^2}{dt^2} \geq 0$$

Stationary state:

$$\frac{ds^2}{dt^2} = 0 \Leftrightarrow \partial_t P = 0$$

Lower bound:

The Cramér-Rao inequality

The Cramér-Rao inequality and the thermodynamic uncertainty relation

The Cramér-Rao inequality

$$\left(\frac{d\langle r\rangle}{dt}\right)^2 \leq \langle \Delta r^2\rangle \frac{ds^2}{dt^2}$$

$r(x)$: observable

$\langle \cdots \rangle = \int dx P(x;t)\ldots$: ensemble average

$\Delta r = r - \langle r \rangle$

A trade-off relationship between a fluctuation $\langle \Delta r^2 \rangle$ and the Fisher information $\frac{ds^2}{dt^2}$

The thermodynamic uncertainty relation

$$\left(\frac{d\langle r\rangle}{dt}\right)^2 \leq \langle (\partial_x r)^2\rangle T\sigma$$

A trade-off relationship between a fluctuation $\langle (\partial_x r)^2 \rangle$ and the entropy production σ

Derivations

The Fokker-Planck equation as the continuity equation

$$\partial_t P(x;t) = -\partial_x(\nu(x;t)P(x;t))$$

Identity $\frac{d\langle r\rangle}{dt} = \int dx P(x;t)\Delta r(\partial_t \ln P(x;t)) = \int dx P(x;t)(\partial_x r(x))\nu(x;t)$

①　②　③

→The Cauchy–Schwarz inequality

The Cramér-Rao inequality

From ① and ②

$$\left(\frac{d\langle r\rangle}{dt}\right)^2 \leq \langle \Delta r^2\rangle\langle(\partial_t \ln P(x;t))^2\rangle = \langle \Delta r^2\rangle\frac{ds^2}{dt^2}$$

The thermodynamic uncertainty relation

From ① and ③

$$\left(\frac{d\langle r\rangle}{dt}\right)^2 \leq \langle(\partial_x r(x))^2\rangle\langle(\nu(x;t))^2\rangle = \langle(\partial_x r)^2\rangle T\sigma$$

A trade-off relationship between the Fisher information and the entropy production

A trade-off relationship between the Fisher information and the entropy production

$$\left(\frac{ds^2}{dt^2}\right)^2 \leq \langle(\partial_x\partial_t \ln P)^2\rangle T\sigma$$

(The Cauchy-Schwartz inequality)

$$\langle(\partial_t \ln P)^2\rangle = \langle(\partial_x\partial_t \ln P)\nu\rangle$$

Equilibrium state ⇒ Stationary state

$$\sigma = 0 \Rightarrow \left(\frac{ds^2}{dt^2}\right) = 0$$

Geodesic and a trade-off relationship between the Fisher information and time

Geodesic

$$\mathcal{L} = \int_{t_{\rm ini}}^{t_{\rm fin}} dt \sqrt{\frac{ds^2}{dt^2}} \geq 2 \arccos \left(\int dx \sqrt{P(x; t_{\rm ini})} \sqrt{P(x; t_{\rm fin})} \right) = \Lambda$$

because

$$ds^2 = \int dx P (d \ln P)^2 = \int dx (2d\sqrt{P(x;t)})^2 \quad 1 = \int dx (\sqrt{P(x;t)})^2$$: Spherical geometry

$$\int dx \sqrt{P(x; t_{\rm ini})} \sqrt{P(x; t_{\rm fin})} = \cos\theta, \mathcal{L} \geq 2\theta$$: Geodesic (Great cycle distance)

i.e., The Bhattacharyya angle

A trade-off relationship between the Fisher information and time (speed limit)

$$(t_{\rm fin} - t_{\rm ini}) \int_{t_{\rm ini}}^{t_{\rm fin}} dt \left(\frac{ds^2}{dt^2} \right) \geq \mathcal{L}^2 \geq \Lambda^2$$

Monotonicity for the relaxation process

The second law of thermodynamics

$$\sigma = \frac{1}{T}\langle \nu^2 \rangle = \frac{1}{T}\langle F\nu \rangle + \frac{d}{dt}\langle -\ln P \rangle \geq 0$$

The Fokker-Planck eq.

$$\partial_t P = -\partial_x(\nu P)$$

$$\nu = F - T\partial_x \ln P$$

Monotonicity of the Fisher information (2nd law-like inequality)

$$\mathcal{I} = \frac{1}{T}\langle (\partial_t \nu)^2 \rangle = \frac{1}{T}\langle (\partial_t F)(\partial_t \nu) \rangle - \frac{1}{2}\frac{d}{dt}\left(\frac{ds^2}{dt^2}\right) \geq 0$$

For the relaxation process

$$\partial_t F = 0 \Rightarrow \frac{d}{dt}\left(\frac{ds^2}{dt^2}\right) \leq 0$$

Monotonically decreasing in time (Relaxation to the stationary state)

Monotonicity and the entropy production

For the relaxation process $\partial_t F = 0$

$$\frac{d}{dt}\left(\frac{ds^2}{dt^2}\right) = -2T\langle(\partial_x \partial_t \ln P)^2\rangle$$

The Fokker-Planck eq.

$$\partial_t P = -\partial_x(\nu P)$$

$$\nu = F - T\partial_x \ln P$$

$$\left(\frac{ds^2}{dt^2}\right) \leq \langle(\partial_x \partial_t \ln P)^2\rangle T\sigma \quad \Rightarrow \quad \frac{d}{dt}\left(\frac{ds^2}{dt^2}\right) \leq -2\frac{\left(\frac{ds^2}{dt^2}\right)^2}{\sigma}$$

An upper bound of the relaxation speed is given by the Fisher information and the entropy production.

$$0 \geq \frac{d}{dt}\left(\frac{ds^2}{dt^2}\right)$$

$$(t_{\rm fin} - t_{\rm ini})\int_{t_{\rm ini}}^{t_{\rm fin}} dt \left(\frac{ds^2}{dt^2}\right) \geq \mathscr{L}^2 \geq \Lambda^2$$

$\Rightarrow$

Speed limit

$$t_{\rm fin} - t_{\rm ini} \geq \frac{\sqrt{2}\Lambda^2}{\sqrt{\frac{ds^2}{dt^2}(t = t_{\rm ini})}\sqrt{\int_{t_{\rm ini}}^{t_{\rm fin}} dt\sigma}}$$

Time derivative of the Fisher information and the excess entropy production

For the master equation

$$\frac{d}{dt}P_i = \sum_j [W_{ij}P_j - W_{ji}P_i]$$

Force: $F_{ij}(P) = W_{ij}P_j - W_{ji}P_i$

Flux: $J_{ij}(P) = \ln \frac{W_{ij}P_j}{W_{ji}P_i}$

Stationary state: $\frac{d}{dt}\bar{P}_i = 0$

$$\delta P_i = P_i - \bar{P}_i$$

The entropy production

$$\sigma = \sum_{i,j|i>j} F_{ij}(P)J_{ij}(P)$$

The excess entropy production (Glansdorff-Prigogine, 1964)

$$\delta^2\sigma = \sum_{i,j|i>j} [F_{ij}(P) - F_{ij}(\bar{P})][J_{ij}(P) - J_{ij}(\bar{P})]$$

The Fisher information

$$\frac{ds^2}{dt^2} = \sum_i \frac{1}{P_i}\left(\frac{dP_i}{dt}\right)^2 = \sum_i P_i \left(\frac{d\ln P_i}{dt}\right)^2$$

$$\delta^2\sigma = -\frac{1}{2}\frac{d}{dt}\left[\sum_i \frac{(\delta P_i)^2}{P_i}\right] \simeq -\frac{1}{2}\frac{d}{dt}[ds^2]$$ around the stationary state

An expansion to chemical reaction networks

Chemical reaction

$$\sum_{i=1}^{N} \nu_{i\rho} X_i \underset{k_\rho^-}{\overset{k_\rho^+}{\rightleftharpoons}} \sum_{i=1}^{N} \kappa_{i\rho} X_i$$

X_i : i-th chemical species ($i = 1, \ldots, N$)
k_ρ^-, k_ρ^+ : rate constants of ρ-th reaction ($\rho = 1, \ldots, M$)
$\nu_{i\rho}, \kappa_{i\rho}$: nonnegative integers
$[X_i]$: X_i 's concentration

The rate equation

$$\frac{d[X_i]}{dt} = \sum_{\rho=1}^{M} (\kappa_{i\rho} - \nu_{i\rho}) \left[k_\rho^+ \prod_{i=1}^{N} [X_i]^{\nu_{i\rho}} - k_\rho^- \prod_{i=1}^{N} [X_i]^{\kappa_{i\rho}} \right]$$

[Deterministic eq.] $[X_i]$ is not a probability in general $\sum_i [X_i] \neq 1$.

The Fisher information for chemical reaction networks

The Fisher information for chemical reaction networks

$$\frac{ds^2}{dt^2} = \sum_i \frac{1}{[\mathrm{X_i}]}\left(\frac{d[\mathrm{X_i}]}{dt}\right)^2 = \sum_i [\mathrm{X}_i]\left(\frac{d\ln[\mathrm{X_i}]}{dt}\right)^2$$

It corresponds to f-divergence of the positive measure space in information geometry.

f-divergence: $D([\mathbf{X}]\|[\mathbf{X}']) = \sum_{i=1}^{N}\left([\mathrm{X_i}]\ln\frac{[\mathrm{X_i}]}{[\mathrm{X_i'}]} - [\mathrm{X_i}] + [\mathrm{X_i'}]\right)$

$$ds^2 = 2D([\mathbf{X}]\|[\mathbf{X}] + d[\mathbf{X}]) + \mathcal{O}(d[\mathbf{X}]^3)$$

cf.) KL divergence for probabilities $\boldsymbol{p}$ and $\boldsymbol{p}'$

$$D_{\mathrm{KL}}([\boldsymbol{p}]\|[\boldsymbol{p}']) = \sum_{i=1}^{N} p_i \ln\frac{p_i}{p_i'} \qquad ds^2 = \sum_i p_i(d\ln p_i)^2 = 2D_{\mathrm{KL}}(\boldsymbol{p}\|\boldsymbol{p} + d\boldsymbol{p}) + \mathcal{O}(d\boldsymbol{p}^3)$$

The Gibbs free energy and the Fisher information

The Gibbs free energy

$$G - G^{\mathrm{eq}} = \sum_i (\mu_i - \mu_i^{\mathrm{eq}})[\mathrm{X}_i] - RT\sum_i [\mathrm{X}_i] + RT\sum_i [\mathrm{X}_i^{\mathrm{eq}}]$$

$$\frac{\partial G}{\partial [\mathrm{X_i}]} = \mu_i = \mu_i^{\circ}(T) + RT\ln[X_i]$$

G (G^{eq}) :The Gibbs free energy (in equilibrium)
μ_i (μ_i^{eq}): i-th chemical potential (in equilibrium)
μ_i° : i-th standard chemical potential
T : temperature
R : gas constant

f-divergence:

$$\Rightarrow \quad \frac{G - G^{\mathrm{eq}}}{RT} = D([\mathbf{X}]||[\mathbf{X}^{\mathrm{eq}}]) = \sum_{i=1}^{N}\left([\mathrm{X_i}]\ln\frac{[\mathrm{X_i}]}{[\mathrm{X_i^{eq}}]} - [\mathrm{X_i}] + [\mathrm{X_i^{eq}}]\right)$$

Fisher information:

$$ds^2 \simeq \frac{2}{RT}(G - G^{\mathrm{eq}})$$

around the equilibrium state

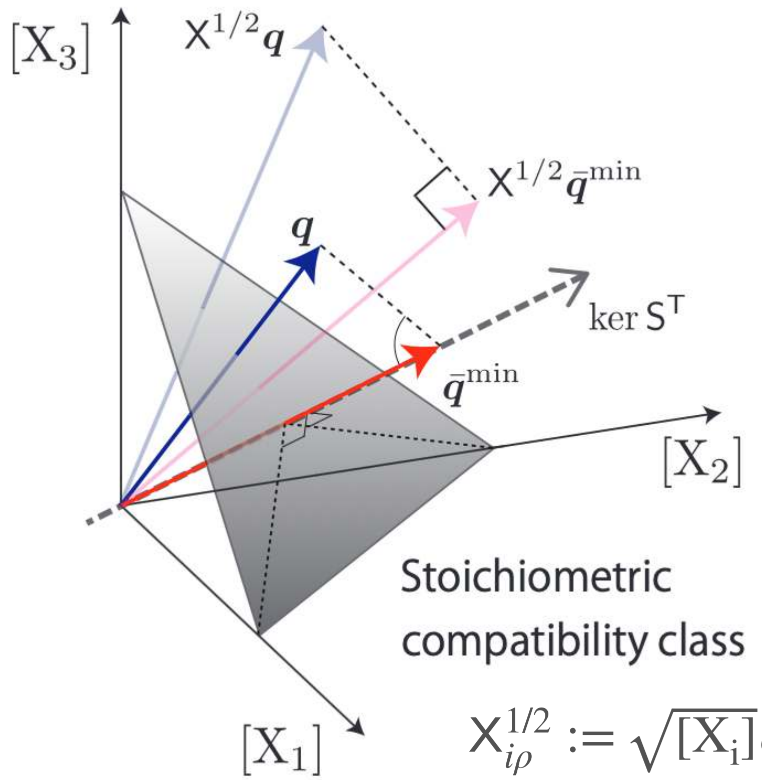
A generalized Cramér-Rao inequality for chemical reaction networks

A generalized Cramér-Rao inequality

$$\left(\frac{d}{dt}\langle\langle \boldsymbol{q} \rangle\rangle\right)^2 \leq \langle\langle (\boldsymbol{q} - \bar{\boldsymbol{q}}^{\min})^2 \rangle\rangle \frac{ds^2}{dt^2}$$

$\langle\langle \cdots \rangle\rangle = \sum_i [X_i] \cdots$: the concentration integral

q_i : $\boldsymbol{i}$-th observable $\qquad \frac{d}{dt}\langle\langle \bar{\boldsymbol{q}}^{\min} \rangle\rangle = 0$



$X^{1/2}_{i\rho} := \sqrt{[X_i]}\delta_{i\rho}$

$\bar{q}_i^{\min}$ is given by the projection onto the kernel of the stoichiometric matrix $S_{i\rho} := \kappa_{i\rho} - \nu_{i\rho}$.

$$\ker S^T := \{\boldsymbol{l} \,|\, S^T \boldsymbol{l} = \boldsymbol{0}\}$$

Stoichiometric comparability class is the set of concentrations that [X] may reach.
cf.) The probability simplex for the master equation

A generalized Cramér-Rao inequality and the speed limit on the Gibbs free energy

The speed limit on the Gibbs free energy

$$\left(\frac{d}{dt}\langle\langle \boldsymbol{q} \rangle\rangle\right)^2 \leq \langle\langle (\boldsymbol{q} - \bar{\boldsymbol{q}}^{\min})^2 \rangle\rangle \frac{ds^2}{dt^2}$$

$$\boldsymbol{q} = \boldsymbol{\mu} \qquad \bar{\boldsymbol{q}}^{\min} = \boldsymbol{\mu}^{\mathrm{eq}}$$

$$\Rightarrow \quad \left|\frac{dG}{dt}\right| \leq \sqrt{\langle\langle (\boldsymbol{\mu} - \boldsymbol{\mu}^{\mathrm{eq}})^2 \rangle\rangle} \sqrt{\frac{ds^2}{dt^2}}$$

The Fisher information and the fluctuation of the chemical potential gives a speed limit for a changing rate of the Gibbs free energy.

cf.) The second law of thermodynamics (for chemical reaction networks) $\quad \dfrac{dG}{dt} \leq 0$

The Brusselator and the speed limit on the Gibbs free energy

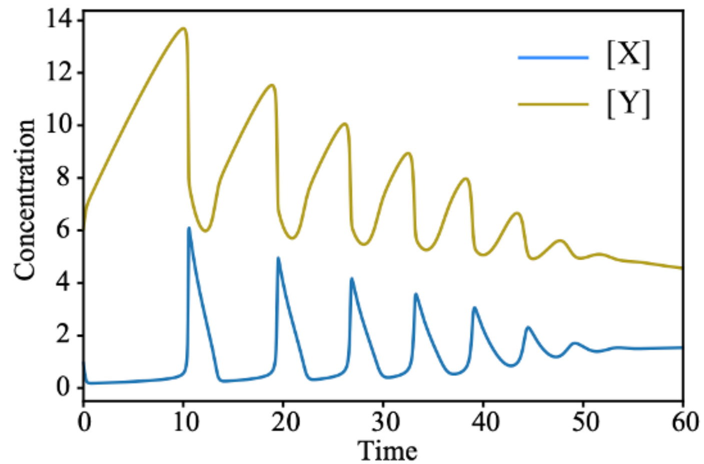
The Brusselator

(A model of oscillating reactions)

$$A \rightleftharpoons X$$

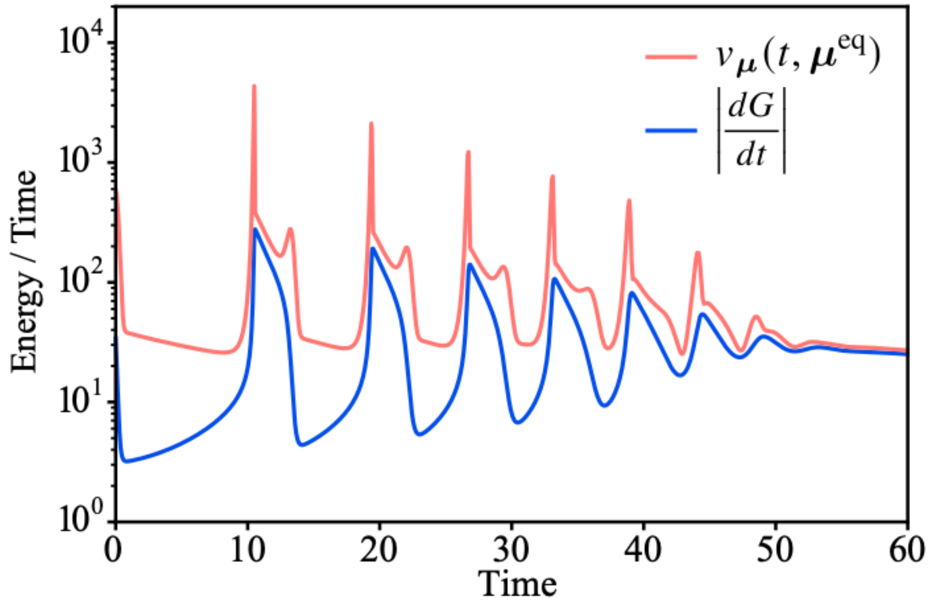
$$2X + Y \rightleftharpoons 3X$$

$$X + B \rightleftharpoons Y + A$$



<u>The speed limit on the Gibbs free energy</u>

$$\left|\frac{dG}{dt}\right| \leq \sqrt{\langle\langle(\boldsymbol{\mu} - \boldsymbol{\mu}^{\mathrm{eq}})^2\rangle\rangle}\sqrt{\frac{ds^2}{dt^2}} = v_{\boldsymbol{\mu}}(t, \boldsymbol{\mu}^{\mathrm{eq}})$$



Summary

We discuss a duality between the Fisher information and the entropy production in stochastic thermodynamics.
The Fisher information gives several variants of thermodynamic uncertainty relations.

Reference:

Stochastic thermodynamic interpretation of information geometry and the trade-off relationship between the Fisher information and time
Sosuke Ito, Phys. Rev. Lett. **121**, 030605. (2018).

A duality between the Fisher information and the entropy production and several variants of thermodynamic uncertainty relations
Sosuke Ito and Andreas Dechant, to appear in Phys. Rev. X (2020). [arXiv 1810.06832 (2018).]

The Fisher information and the excess entropy production by Glansdorff and Prigogine
Sosuke Ito, arXiv 1908.09446 (2019).

A generalized Cramér-Rao inequality for chemical reaction networks
Kohei Yoshimura and Sosuke Ito, arXiv 2005.08444 (2020).


Andreas Dechant


Kohei Yoshimura

Universal Biology Institute

PRESTO sakigake

Information physics of living matters

Thank you for your attention!