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

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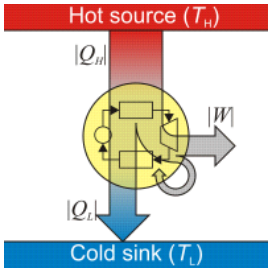
<u>Reference</u>

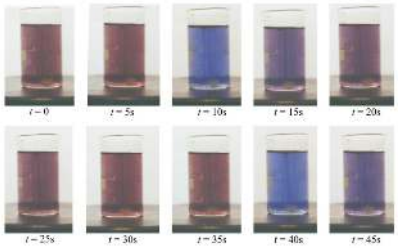
Sosuke Ito, Phys. Rev. Lett. **121**, 030605. (2018).
Sosuke Ito and Andreas Dechant, to appear in Phys. Rev. X (2020). [arXiv 1810.06832 (2018).]
Sosuke Ito, arXiv 1908.09446 (2019).
Kohei Yoshimura and Sosuke Ito, arXiv 2005.08444 (2020).

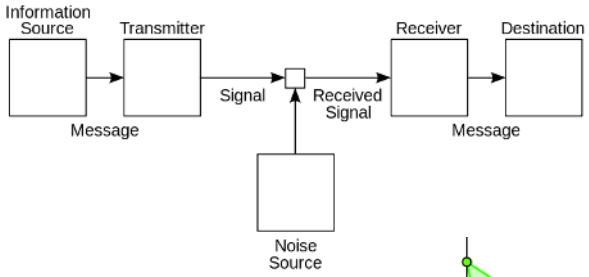
Concept

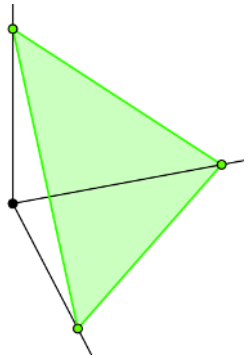
- **A unified theory of thermodynamics and information**

Thermodynamics ⟷ Information theory (Information geometry)









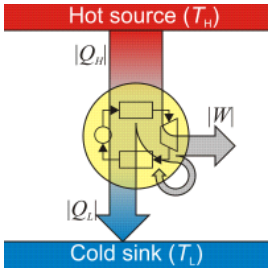
(Pictures from Wikipedia)

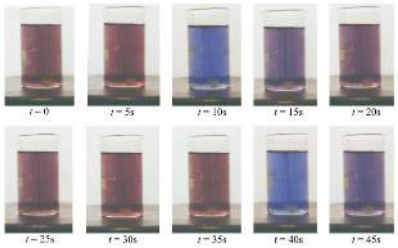
Concept

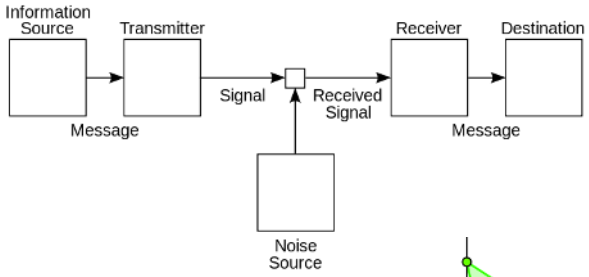
Two key concepts

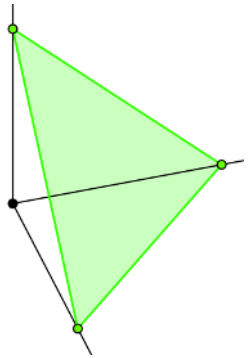
- **A unified t**

Thermodynamics ⟷ Information theory (Information geometry)









(Pictures from Wikipedia)

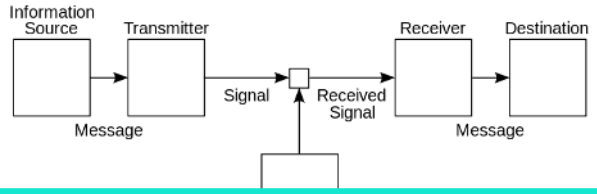
Concept

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 $$\underset{①}{\frac{d\langle r\rangle}{dt}} = \underset{②}{\int dx P(x;t)\Delta r(\partial_t \ln P(x;t))} = \underset{③}{\int dx P(x;t)(\partial_x r(x))\nu(x;t)}$$

→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

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

because

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

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

i.e., The Bhattacharyya angle

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

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

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 $\partial_t F = 0$

The Fokker-Planck eq.

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

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

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

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

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

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

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
$[\mathrm{X}_i]$: X_i 's concentration

The rate equation

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

[Deterministic eq.] $[\mathrm{X}_i]$ is not a probability in general $\sum_i [\mathrm{X}_i] \neq 1$.

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

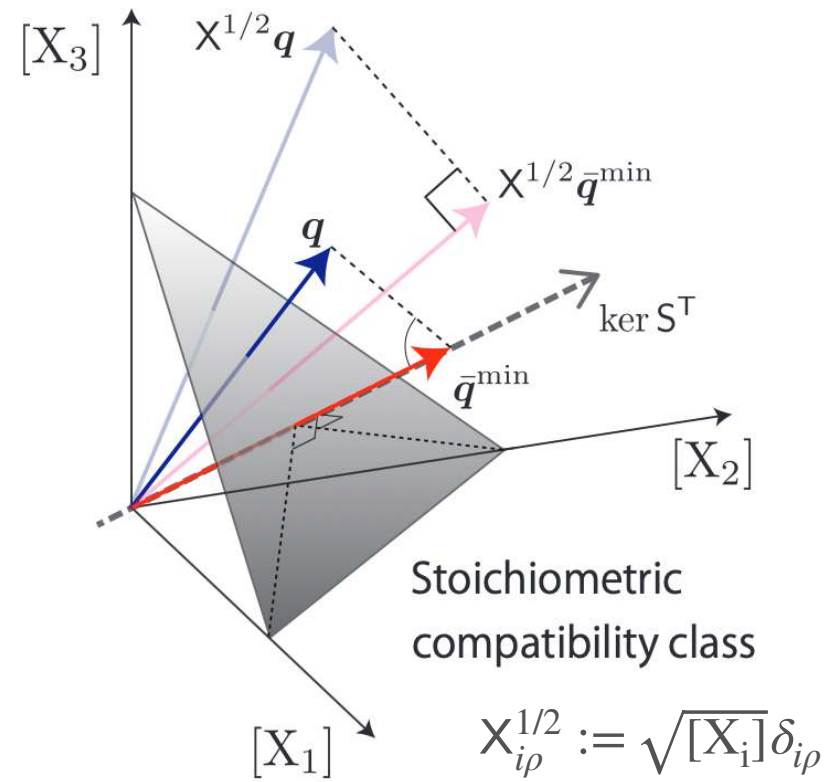
A generalized Cramér-Rao inequality

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

$\langle\langle\cdots\rangle\rangle = \sum_i [\mathrm{X}_i]\cdots$: the concentration integral

q_i : i-th observable

$$\frac{d}{dt}\langle\langle \bar{\boldsymbol{q}}^{\min}\rangle\rangle = 0$$



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

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

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

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) $\dfrac{dG}{dt} \leq 0$

The Brusselator and the speed limit on the Gibbs free energy

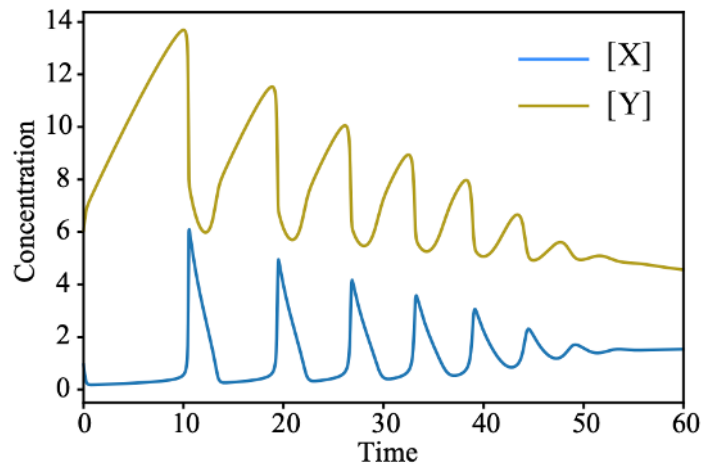
The Brusselator

(A model of oscillating reactions)

$$A \rightleftharpoons X$$

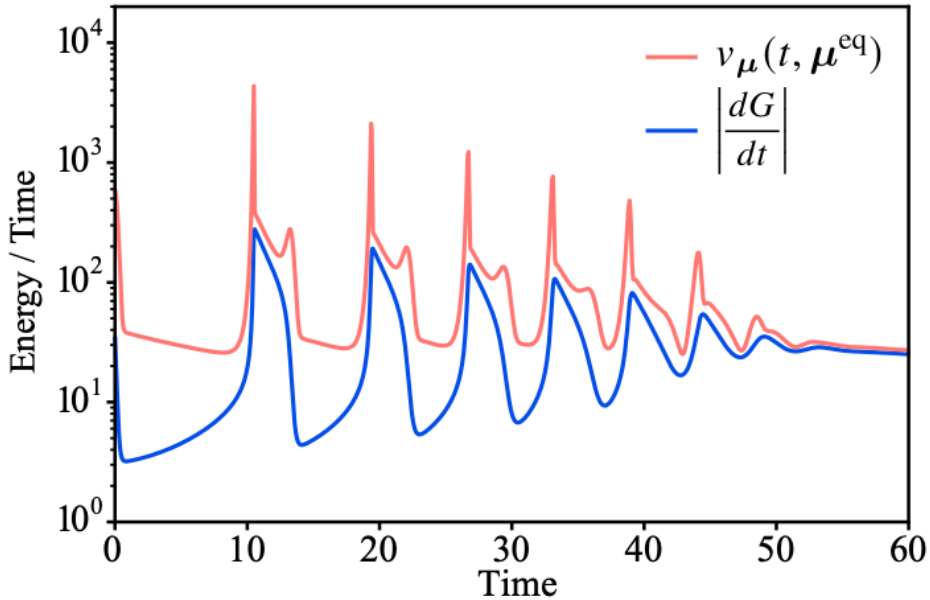
$$2X + Y \rightleftharpoons 3X$$

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



<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
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Andreas Dechant

Kohei Yoshimura

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Thank you for your attention!