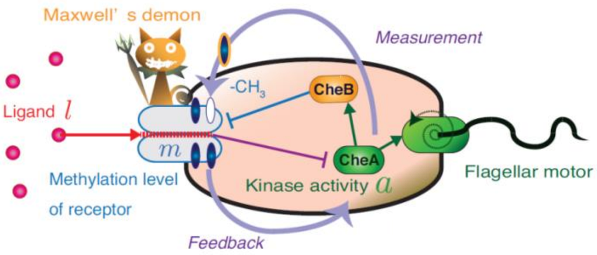
Thermodynamics of Autonomous Information Processing



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KIAS Workshop on Quantum Information and Thermodynamics

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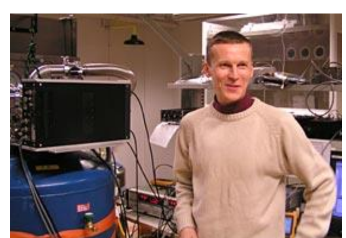

Outline

- Introduction
- Information thermodynamics on causal networks
- Application to biochemical signal transduction
- Summary

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- **Introduction**
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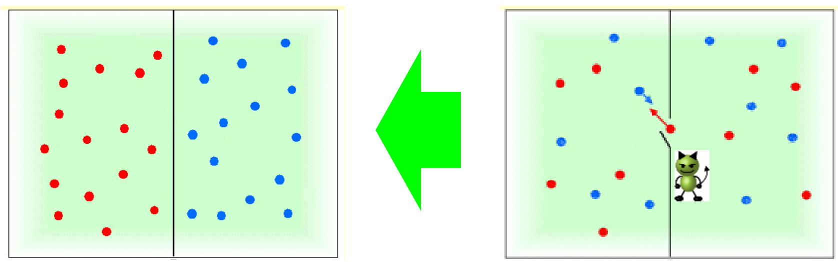
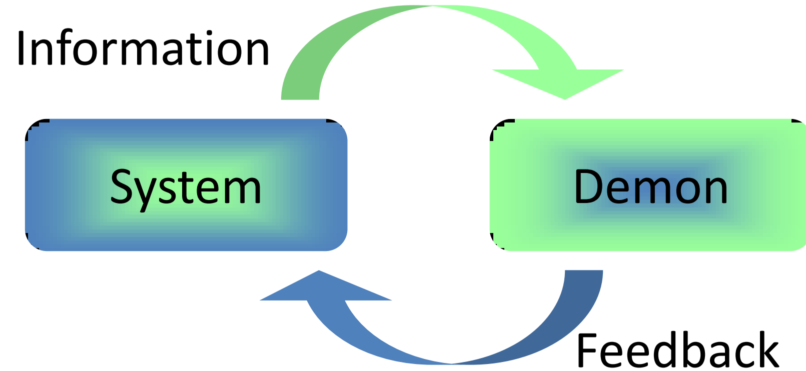
Information Thermodynamics





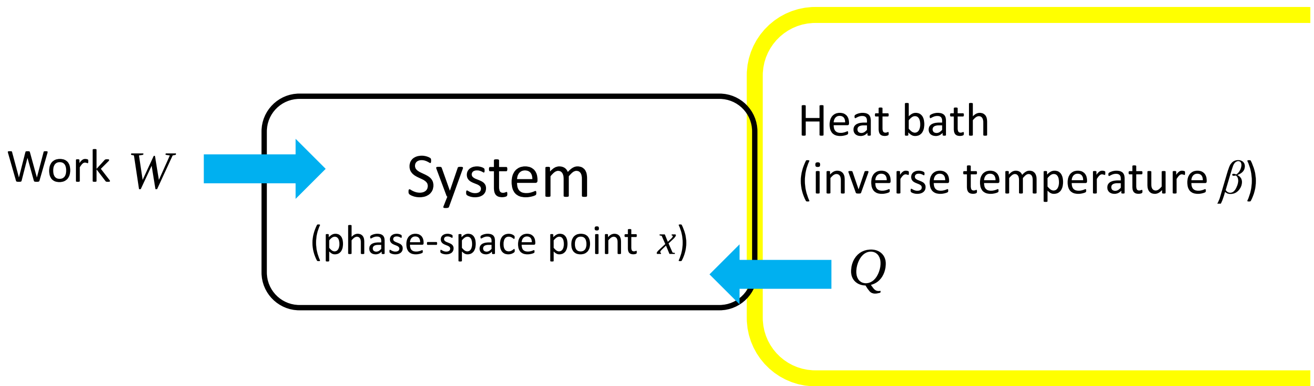
Information processing at the level of thermal fluctuations

✓ Foundation of the second law of thermodynamics

✓ Application to nanomachines and nanodevices

Review: J. M. R. Parrondo, J. M. Horowitz, & T. Sagawa, *Nature Physics* **11**, 131-139 (2015).

Stochastic Entropy Production



Stochastic entropy production along a trajectory of the system from time 0 to τ

$$\Delta s_{\mathrm{SB}} \equiv \Delta s_{\mathrm{S}} - \beta Q$$

$$\Delta s_{\mathrm{S}} \equiv s_{\mathrm{S}}[x(\tau),\tau] - s_{\mathrm{S}}[x(0),0] \qquad s_{\mathrm{S}}[x,t] \equiv -\ln P[x,t]$$

$$\langle \Delta s_{\mathrm{S}} \rangle = \Delta S_{\mathrm{S}}$$

$P[x,t]$: probability distribution at time t

If the initial and the final states are canonical distributions: $\Delta s_{\mathrm{SB}} = \beta (W - \Delta F)$

Integral Fluctuation Theorem and Jarzynski Equality

Integral fluctuation theorem

$$\left\langle e^{-\Delta s_{\mathrm{SB}}} \right\rangle = 1$$

Seifert, PRL (2005), …

for any initial and final distributions

Second law can be expressed by an **equality** with full cumulants

⇒ The second law of thermodynamics (Clausius inequality)

$$\left\langle \Delta s_{\mathrm{SB}} \right\rangle \geq 0 \quad \Leftrightarrow \quad \Delta S_{\mathrm{S}} \geq \beta \langle Q \rangle$$

Jarzynski equality

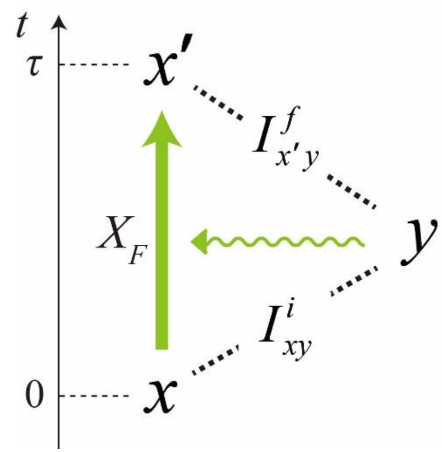
Jarzynski, PRL (1997)

$$\Delta s_{\mathrm{SB}} = \beta (W - \Delta F) \quad \Rightarrow \quad \left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F} \quad \Rightarrow \quad \langle W \rangle \geq \Delta F$$

General Principle of Information Thermodynamics

$$\left\langle e^{-\Delta s_{\mathrm{XB}}+\Delta I} \right\rangle = 1$$

$$\Rightarrow \quad \langle \Delta s_{\mathrm{XB}} \rangle \geq \langle \Delta I \rangle$$



Feedback:

$$\left\langle e^{-\Delta s_{\mathrm{XB}}+(I_{\mathrm{rem}}-I)} \right\rangle = 1$$

$$\Rightarrow \quad \langle \Delta s_{\mathrm{XB}} \rangle \geq -\langle I - I_{\mathrm{rem}} \rangle$$

Measurement:

$$\left\langle e^{-\Delta s_{\mathrm{XB}}+I} \right\rangle = 1$$

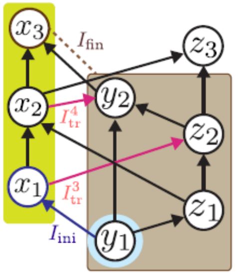
$$\Rightarrow \quad \langle \Delta s_{\mathrm{XB}} \rangle \geq \langle I \rangle$$

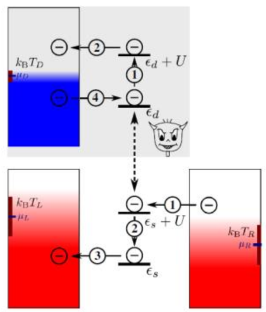
Unified formulation of measurement and feedback

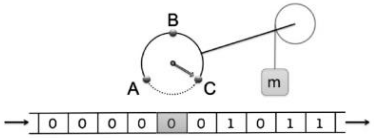
TS and M. Ueda, PRL **109**, 180602 (2012).

Thermodynamics of Autonomous Information Processing

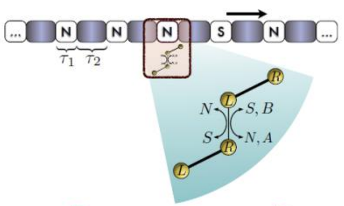
- **Second law & fluctuation theorem**
  Allahverdyan, Dominik & Guenter, J. Stat. Mech. (2009)
  Hartich, Barato, & Seifert, J. Stat. Mech. (2014)
  Horowitz & Esposito, Phys. Rev. X (2014)
  Horowitz & Sandberg, New J. Phys. (2014)
  Shiraishi & Sagawa, Phys. Rev. E (2015)
  Ito & Sagawa, Phys. Rev. Lett. (2013)

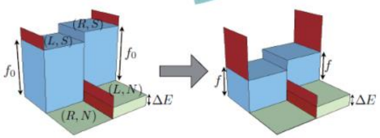






- **Models of autonomous Maxwell's demons**
  Mandal & Jarzynski, PNAS (2012)
  Mandal, Quan, & Jarzynski, Phys. Rev. Lett. (2013)
  Strasberg, Schaller, Brandes, & Esposito Phys. Rev. Lett. (2013)
  Horowitz, Sagawa, & Parrondo, Phys. Rev. Lett. (2013)
  Shiraishi, Ito, Kawaguchi & Sagawa, New J. Phys. (2015)





Toward deeper understanding of information nanomachines

Two Approaches

- **"Transfer entropy"** approach
  - ✓ Applicable to non-Markovian dynamics
  - ✓ Second law is weaker in Markovian dynamics

Ito & Sagawa, Phys. Rev. Lett. (2013)

- **"Information flow"** approach
  - ✓ Not applicable to non-Markovian dynamics
  - ✓ Second law is stronger in Markovian dynamics

Second law: Allahverdyan, Dominik & Guenter, J. Stat. Mech. (2009)
Hartich, Barato, & Seifert, J. Stat. Mech. (2014)
Horowitz & Esposito, Phys. Rev. X (2014)
Horowitz & Sandberg, New J. Phys. (2014)

Fluctuation theorem: Shiraishi & Sagawa, PRE (2015)

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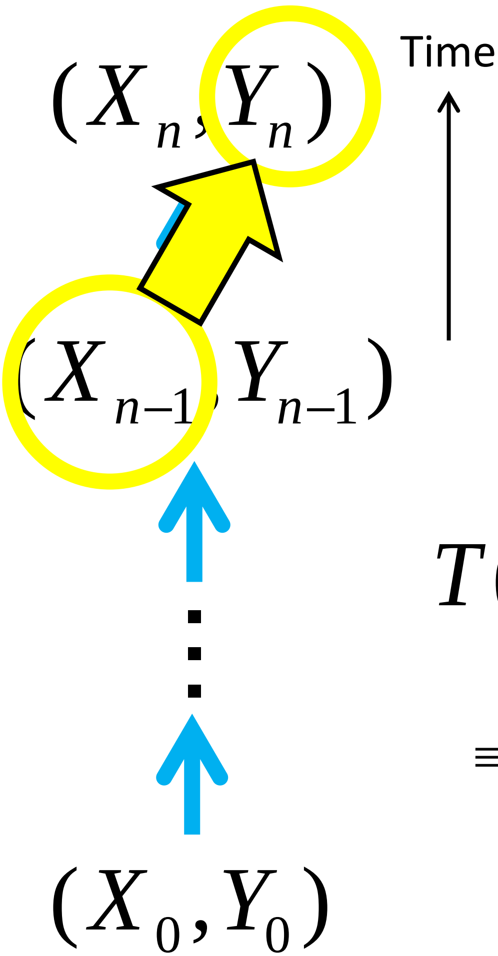
Transfer Entropy (1)

Stochastic dynamics of a bipartite system



Transfer entropy:
Directional information flow
from X to Y
during time n and $n+1$

Conditional mutual information

$$T(X_{n-1} \to Y_n) \equiv I\left(X_{n-1} : Y_n \mid Y_{n-1} \cdots Y_0\right)$$

$$\equiv \sum_{x_{n-1}, y_0, \cdots y_n} p(x_{n-1}, y_0, \cdots y_n) \ln \frac{p(x_{n-1}, y_n \mid y_0, \cdots y_{n-1})}{p(x_{n-1} \mid y_0, \cdots y_{n-1})\, p(y_n \mid y_0, \cdots y_{n-1})}$$

T. Schreiber, PRL **85**, 461 (2000)

Transfer Entropy (2)

(X_1, Y_1)

↑

(X_0, Y_0)

Example: Two bit system

$x_1 = x_0 \qquad y_1 = x_0 \oplus y_0$ **(CNOT gate)**

Binary sum

$$T(X_0 \to Y_1) \equiv I\left(X_0 : Y_1 \mid Y_0\right)$$

$x_0 = 0 \text{ or } 1$

(with probability 1/2)

$y_0 = 0$

⇒ $y_1 = x_0$

Time-delayed mutual information

$$I\left(X_0 : Y_1\right) = \ln 2$$

$$T(X_0 \to Y_1) = \ln 2$$

$x_0 = 0 \text{ or } 1$

$y_0 = 0 \text{ or } 1$

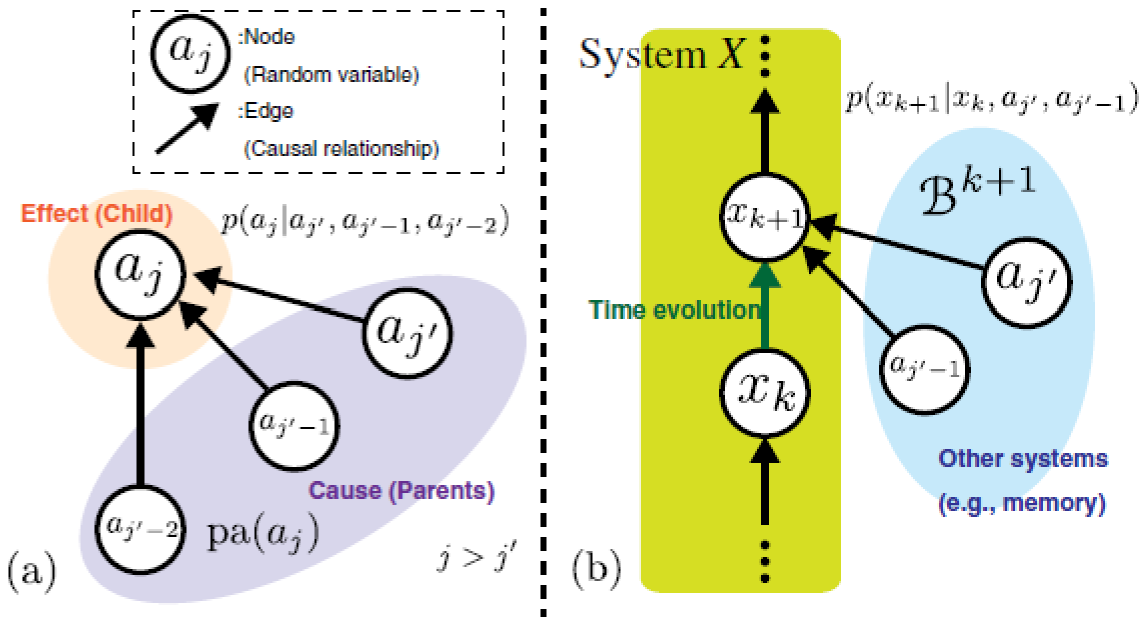
(with probability 1/2, no correlation)

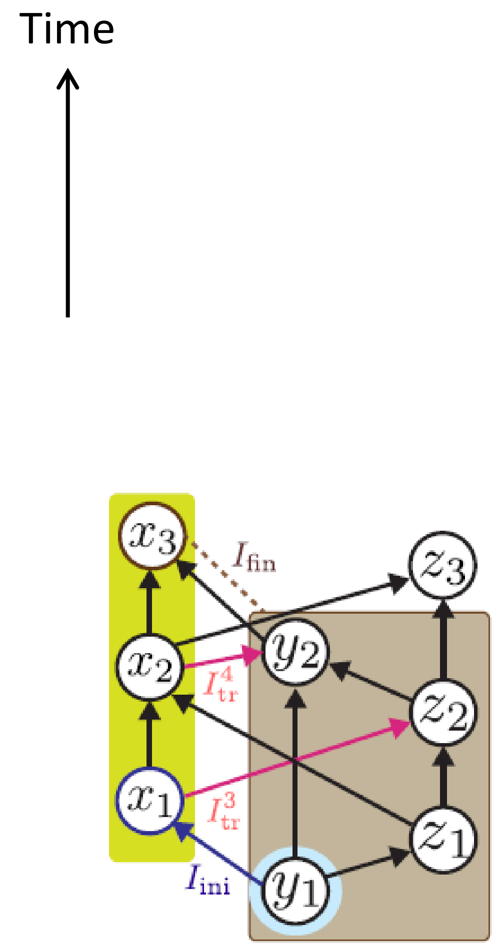
⇒

$$I\left(X_0 : Y_1\right) = 0$$

$$T(X_0 \to Y_1) = \ln 2$$

Many-body Systems with Complex Information Flow

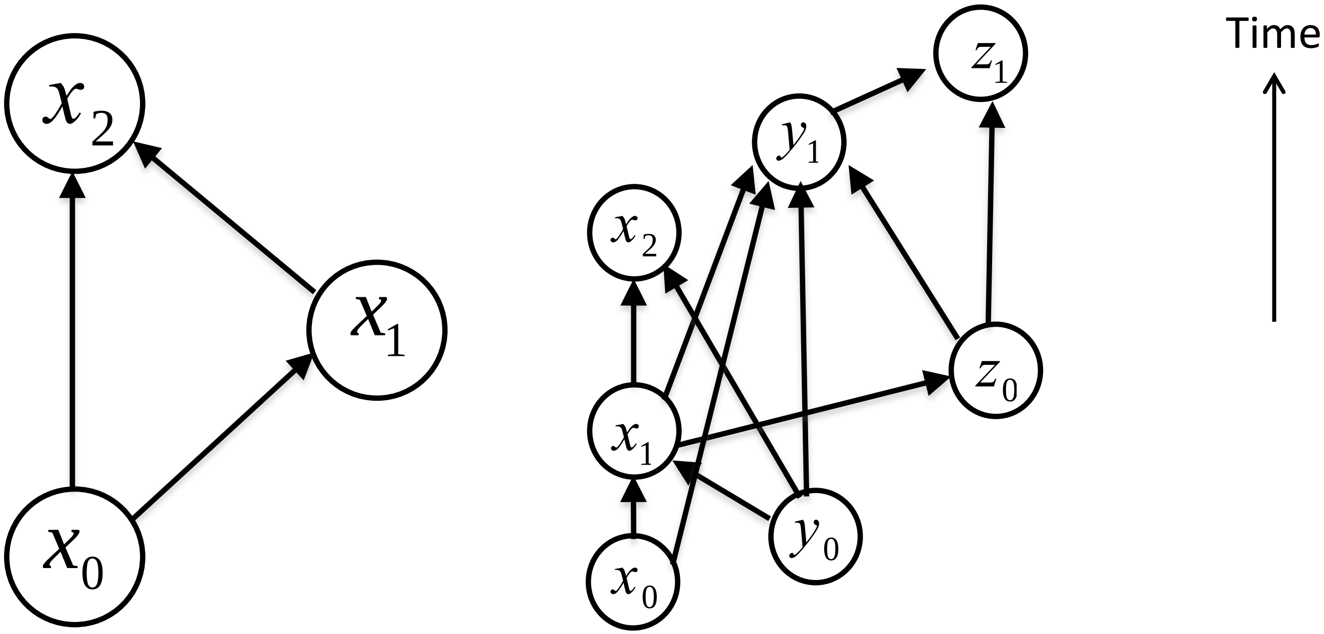




Characterize the dynamics by **Bayesian networks**

Sosuke Ito & TS, PRL 111, 180603 (2013).

Bayesian Networks



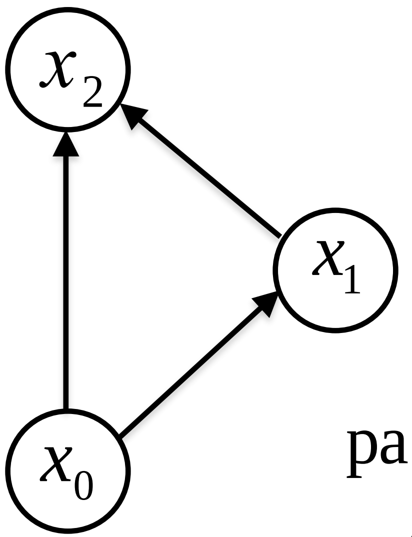
Node: Event

Arrow: Causal relationship

Parents of Nodes

Parents of node x (denoted by "$\mathrm{pa}(x)$"):

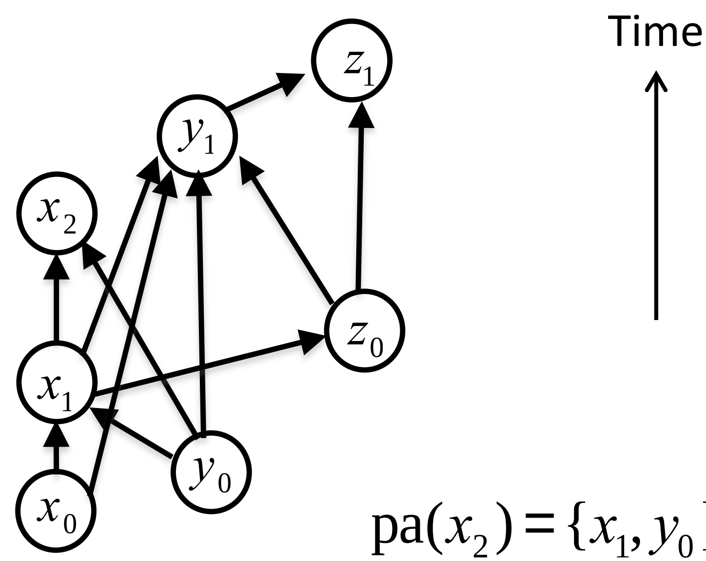
The set of nodes that have arrows to x



$$\mathrm{pa}(x_1) = \{x_0\}$$

$$\mathrm{pa}(x_2) = \{x_1, x_0\}$$

$$\mathrm{pa}(x_0) = \text{Æ}$$



$$\mathrm{pa}(x_2) = \{x_1, y_0\}$$

$$\mathrm{pa}(x_1) = \{x_0, y_0\}$$

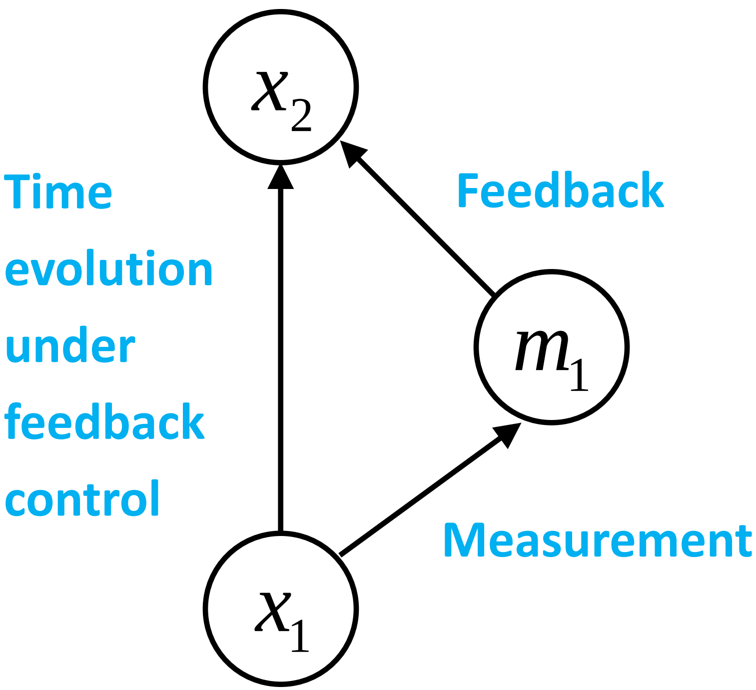
$$\mathrm{pa}(y_1) = \{x_1, x_0, y_0, z_0\}$$

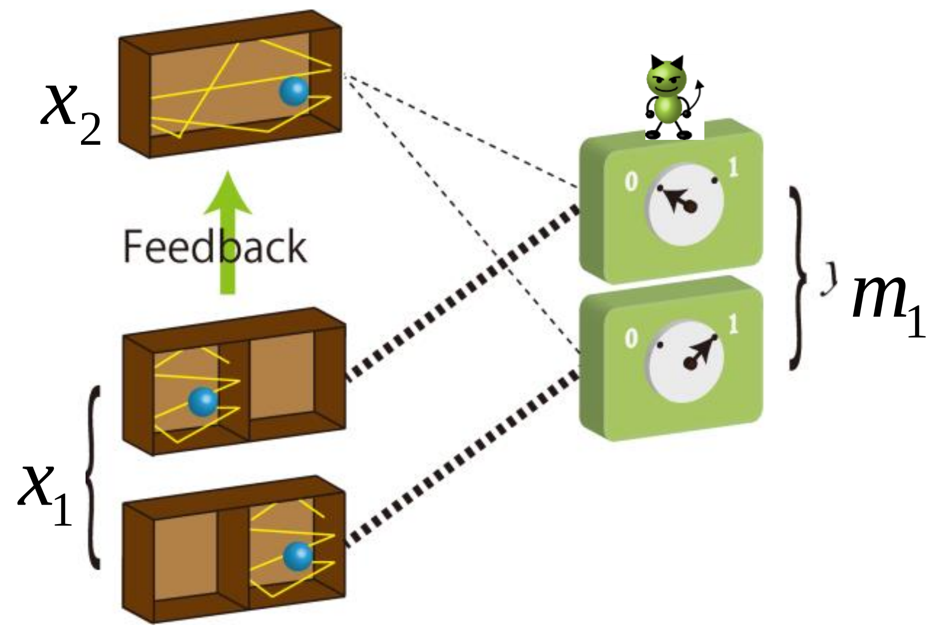
$$\vdots$$

Example: Measurement and Feedback

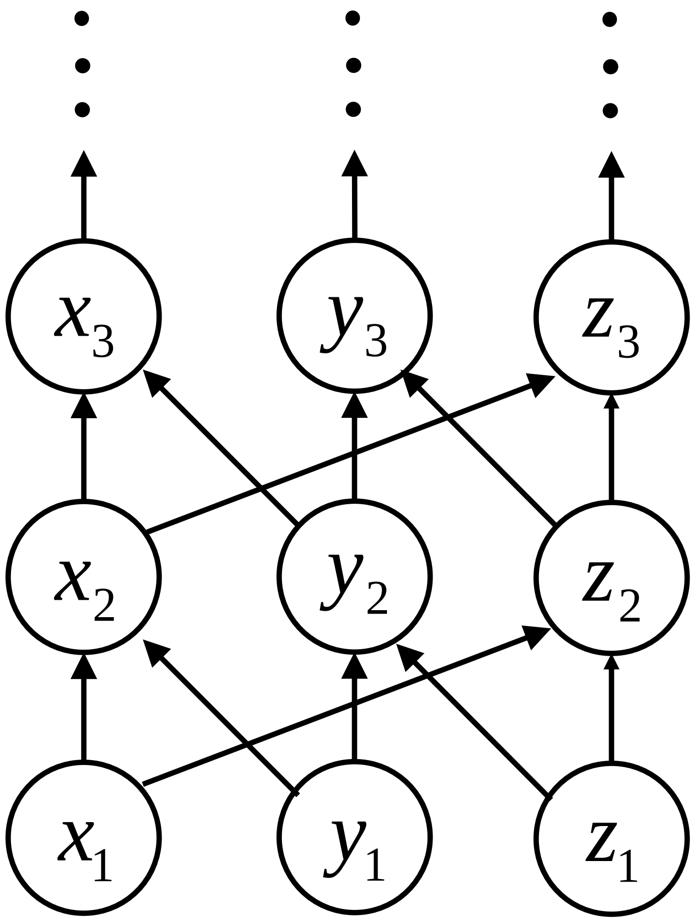
The path probability

$$p(x_1)\,p(m_1 \mid x_1)\,p(x_2 \mid m_1, x_1)$$





Multidimensional Langevin Dynamics



$$x_{i+1} = x_i + f_x\left(x_i, y_i\right)dt + x_x dt$$

$$x_i \equiv x(t = idt) \quad y_i \equiv y(t = idt)$$

$$z_i \equiv z(t = idt)$$

$$\frac{dx}{dt} = f_x\left(x, y\right) + \xi_x$$

$$\frac{dy}{dt} = f_y\left(y, z\right) + \xi_y$$

$$X = x, y, z$$

$$\frac{dz}{dt} = f_z\left(z, x\right) + \xi_z$$

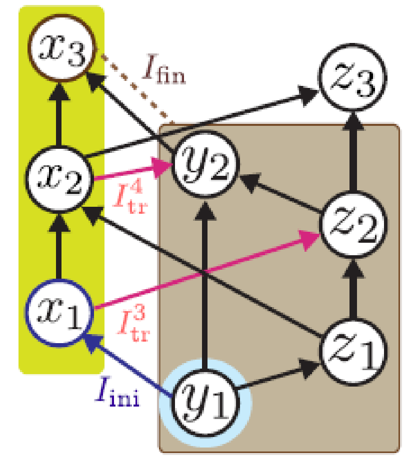
$$\left\langle x_X(t) \right\rangle = 0,$$

$$\left\langle x_X\left(t\right) x_{X'}(t') \right\rangle = D_X d_{XX'} d(t - t')$$

Main Result

$$\left\langle \exp[-\Delta s_{\mathrm{XB}} + \Theta] \right\rangle = 1, \ \left\langle \Delta s_{\mathrm{XB}} \right\rangle \geq \left\langle \Theta \right\rangle$$

$$\Theta = I_{\mathrm{fin}} - I_{\mathrm{ini}} - \sum_{l} I_{\mathrm{tr}}^{l}$$



$\Delta s_{\mathrm{XB}} = \Delta s_{\mathrm{X}} - \beta Q_{\mathrm{X}}$ **: Entropy production in X and the bath**

I_{ini} : Initial correlation between X and the other systems

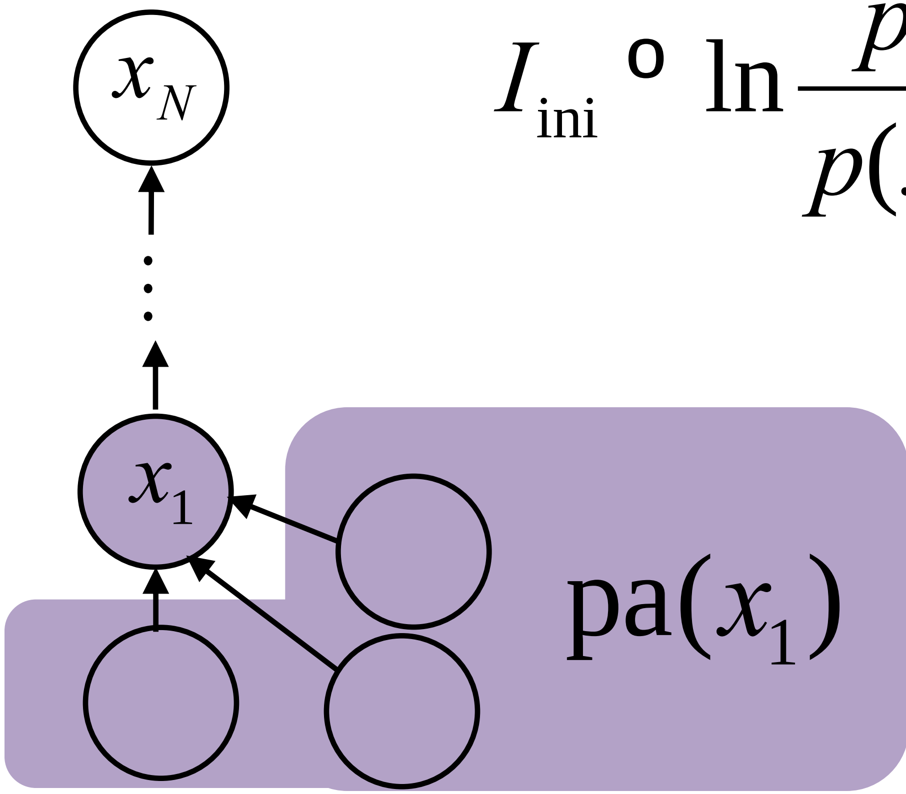
I_{fin} : Final correlation between X and the other systems

I_{tr}^{l}: Transfer entropy from X to the other systems during the dynamics

Sosuke Ito & TS, PRL 111, 180603 (2013).

I_{ini}: Initial Correlation

Initial correlation between X and the other systems

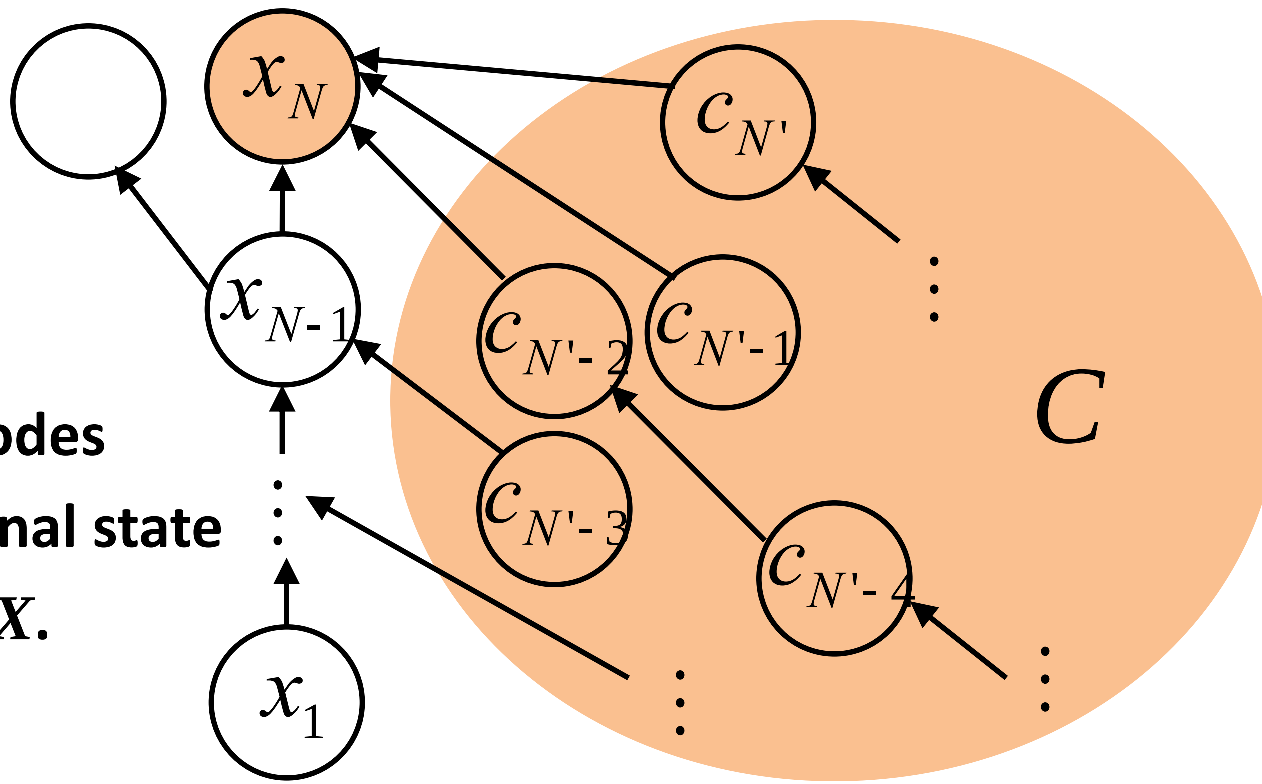


$$I_{\text{ini}} \equiv \ln \frac{p(x_1, \text{pa}(x_1))}{p(x_1)\,p(\text{pa}(x_1))}$$

I_{fin}: Final Correlation

Final correlation between X and the other systems

$$I_{\text{fin}} \circ \ln \frac{p(x_N, C)}{p(x_N)p(C)}$$



C **is the set of nodes that affect the final state from outside of** ***X*****.**

I^l_{tr} : Transfer entropy

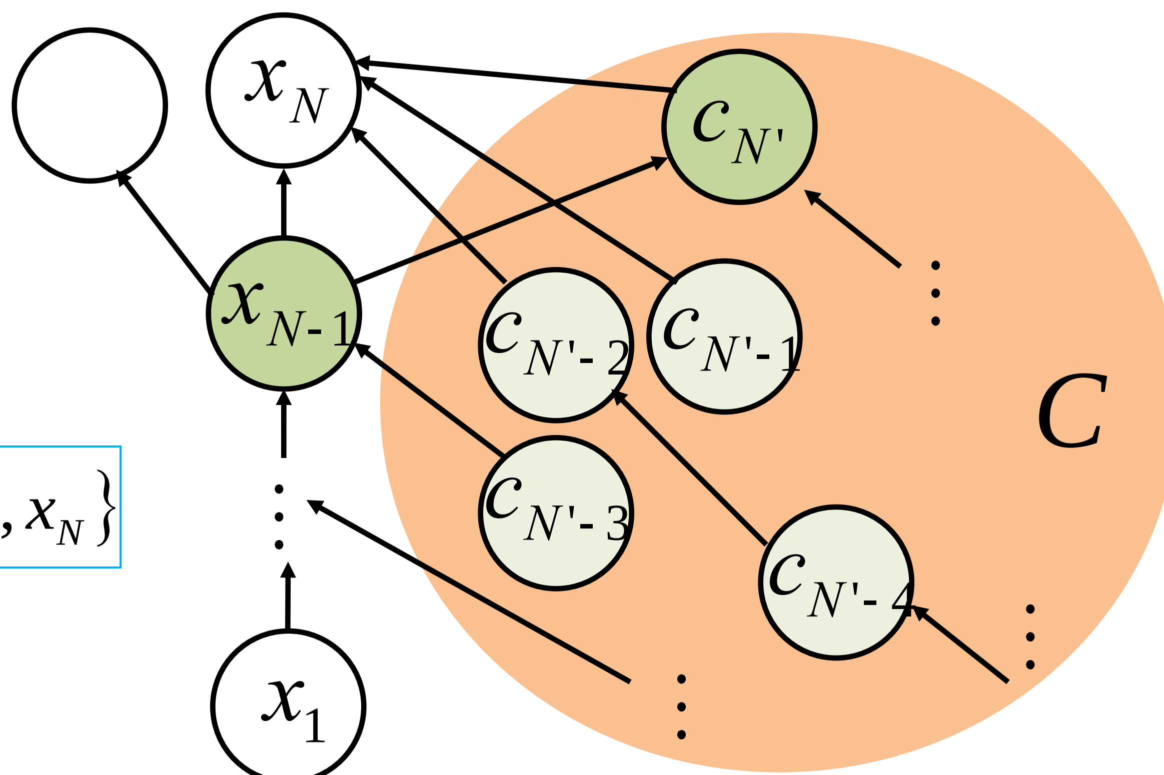
Transfer entropy from *X* to c_l during the dynamics

$$I^l_{\mathrm{tr}} \equiv \ln \frac{p(\mathrm{pa}_X(c_l), c_l \mid c_{l-1}, \ldots, c_1)}{p(c_l \mid c_{l-1}, \ldots, c_1)\, p(\mathrm{pa}_X(c_l) \mid c_{l-1}, \ldots, c_1)} \qquad (l = 1, \ldots, N)$$

$$C = \{ c_l \mid 1 \leq l \leq N' \}$$

↑Topological ordering

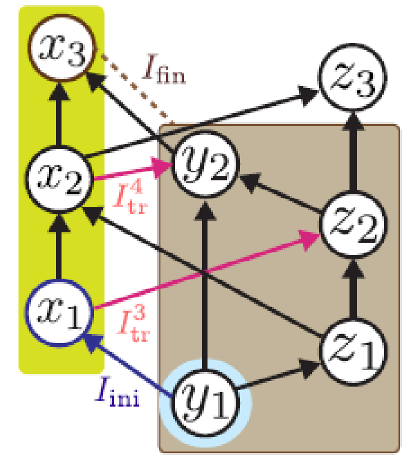
$$\mathrm{pa}_X(c_l) \equiv \mathrm{pa}(c_l) \cap \{x_1, \ldots, x_N\}$$



Main Result

$$\langle \exp[-\Delta s_{\rm XB} + \Theta] \rangle = 1, \ \langle \Delta s_{\rm XB} \rangle \geq \langle \Theta \rangle$$

$$\Theta = I_{\rm fin} - I_{\rm ini} - \sum_l I_{\rm tr}^l$$



$\Delta s_{\rm XB} = \Delta s_{\rm X} - \beta Q_{\rm X}$ **: Entropy production in X and the bath**

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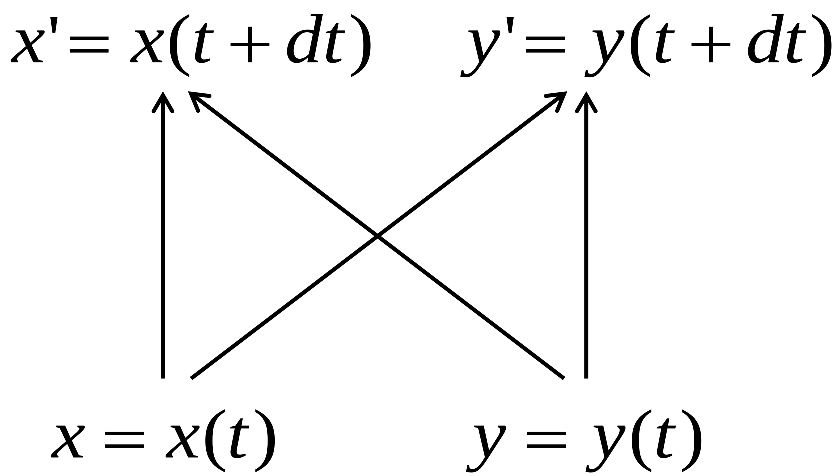
Sosuke Ito & TS, PRL 111, 180603 (2013).

Coupled Langevin System

Infinitesimal transition



$$\dot{x}(t) = f(x(t), y(t)) + \xi_x(t)$$

$$\dot{y}(t) = g(x(t), y(t)) + \xi_y(t)$$

$\langle \xi_x(t) \xi_y(t) \rangle = 0$: independent noise

2nd law: $\langle s(x') - s(x) - \beta Q \rangle \geq \langle I(x' : y') - I(x : y) - \underline{I(x : y' | y)} \rangle$

Transfer entropy

$\Leftrightarrow$ $\langle s(x' | y') - s(x | y) - \beta Q \rangle \geq -\underline{\langle I(x : y' | y) \rangle}$

Cf. $\langle s(x') - s(x) - \beta Q \rangle \geq \underline{\langle I(x' : y) - I(x : y) \rangle}$

Information flow

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Toward Biological Information Processing

What is the role of information in living systems?

Mutual information is experimentally accessible

ex. Apoptosis path: Cheong *et al*. *Science* (2011).

There is no explicit channel coding inside living cells;

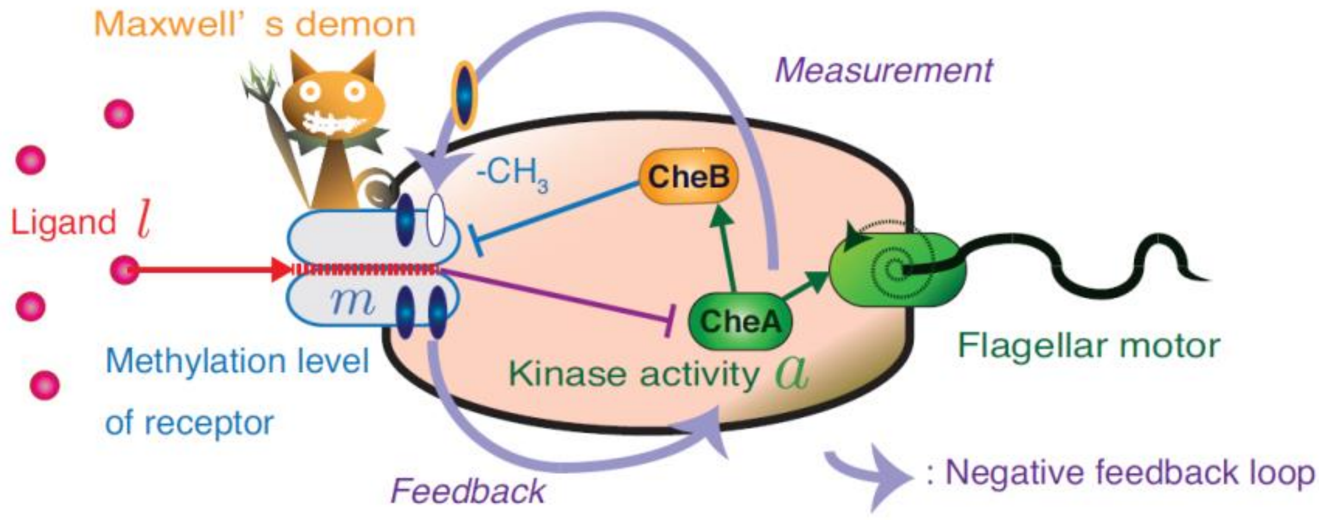
Shannon's second theorem is not straightforwardly applicable

➡ **Application of information thermodynamics**

Barato, Hartich & Seifert, New J. Phys. **16**, 103024 (2014).
Sartori, Granger, Lee & Horowitz, PLoS Compt. Biol. **10**, e1003974 (2014).
Ito & Sagawa, Nat. Commu. **6**, 7498 (2015).
Ouldridge, Govern, & Rein ten Wolde, arXiv:1503.00909 (2015).

Our finding:
Relationship between information and the robustness of adaptation

Signal Transduction of *E. Coli* Chemotaxis



E. Coli moves toward food (ligand)

The information about **ligand density** is transferred to the **methylation level** of the receptor, and used for the feedback to the **kinase activity**.

Adaptation Dynamics

2D Langevin model

Y. Tu *et al., Proc. Natl. Acad. Sci. USA* **105**, 14855 (2008).
F. Tostevin and P. R. ten Wolde, *Phys. Rev. Lett.* **102**, 218101 (2009).
F. G. Lan *et al., Nature Physics* **8**, 422 (2012).

$$\dot{a}_t = -\frac{1}{\tau^a}[a_t - \bar{a}_t(m_t, l_t)] + \xi_t^a$$

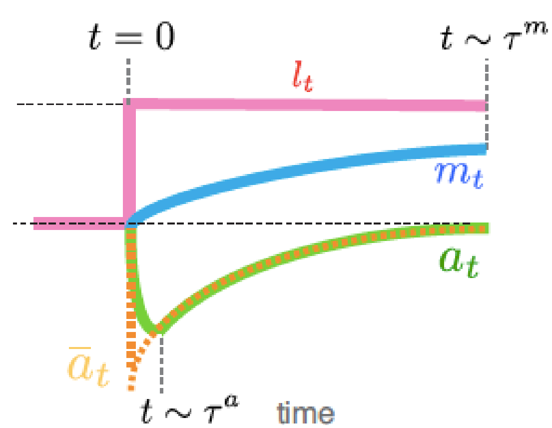
$$\dot{m}_t = -\frac{1}{\tau^m} a_t + \xi_t^m$$

$$\langle \xi_t^x \rangle = 0 \quad \langle \xi_t^x \xi_{t'}^{x'} \rangle = 2T_t^x \delta_{xx'} \delta(t - t')$$

$\bar{a}_t(m_t, l_t) \simeq \alpha m_t - \beta l_t$: stationary value of a_t

$\alpha, \beta > 0$

a_t : kinase activity
m_t : methylation level
l_t : average ligand density
$\tau^m \gg \tau^a > 0$: time constants



Negative feedback loop:

- ✓ Instantaneous change of a_t in response to l_t
- ✓ Memorize l_t by m_t
- ✓ a_t goes back to the initial value

Second Law of Information Thermodynamics

$$dI_t^{\rm tr} + dS_t^{a|m} \geq \frac{J_t^a}{T_t^a} dt$$

(Weaker version with transfer entropy)

$dS_t^{a|m} := \langle \ln p(a_t|m_t) \rangle - \langle \ln p(a_{t+dt}|m_{t+dt}) \rangle$: Change in the conditional Shannon entropy

$dI_t^{\rm tr} := I(a_t : m_{t+dt}|m_t)$ **: Transfer entropy**

$\frac{J_t^a}{T_t^a} = \frac{1}{\tau^a T_t^a} \left[T_t^a - \frac{\langle (a_t - \bar{a}_t)^2 \rangle}{\tau^a} \right]$ **: Robustness against the environmental noise**

Upper bound of the robustness is given by the transfer entropy

S. Ito & T. Sagawa, *Nature Communications* **6**, 7498 (2015).

Stationary State

$$\langle (a_t - \bar{a}_t)^2 \rangle \geq \tau^a T_t^a \left[1 - \frac{dI_t^{\mathrm{tr}}}{dt} \right]$$

Fluctuation (inaccuracy of information transmission) induced by environmental noise

Transfer entropy

Without feedback： $\langle (a_t - \bar{a}_t)^2 \rangle \geq \tau^a T_t^a$

Exact Expression of Transfer Entropy

If the Langevin equation is linear:

$$dI_t^{\mathrm{tr}} = \frac{1}{2} \ln \left(1 + \frac{dP_t}{N_t} \right)$$

Signal-to-noise ratio

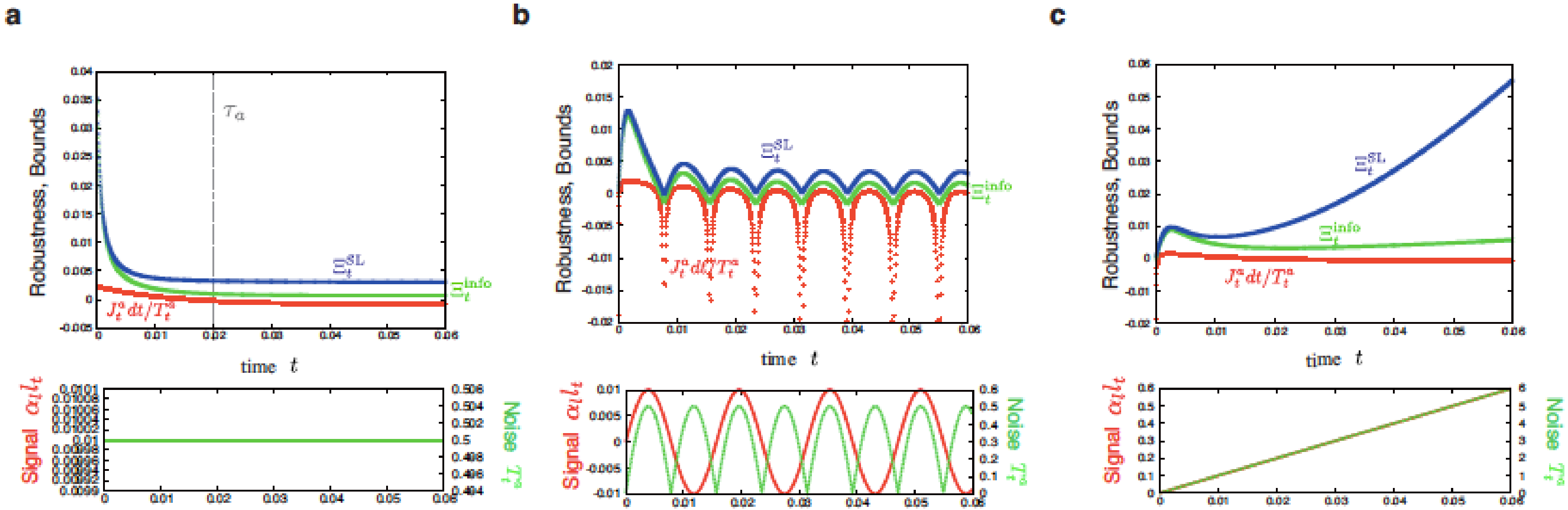
$$dP_t := \frac{(\rho_t^{am})^2 V_t^a}{(\tau^m)^2} dt$$ **: power of the signal from *a* to *m***

$$N_t := 2T_t^m$$ **: noise of *m***

$$V_t^x := \langle x_t^2 \rangle - \langle x_t \rangle^2 \qquad \rho_t^{am} := \frac{\langle a_t m_t \rangle - \langle a_t \rangle \langle m_t \rangle}{\sqrt{V_t^a V_t^m}}$$

Analogous to the Shannon–Hartley theorem

Information-Thermodynamic Efficiency



Input ligand signal: a, step function. b, sinusoidal function. c, linear function.

Numerical simulation:

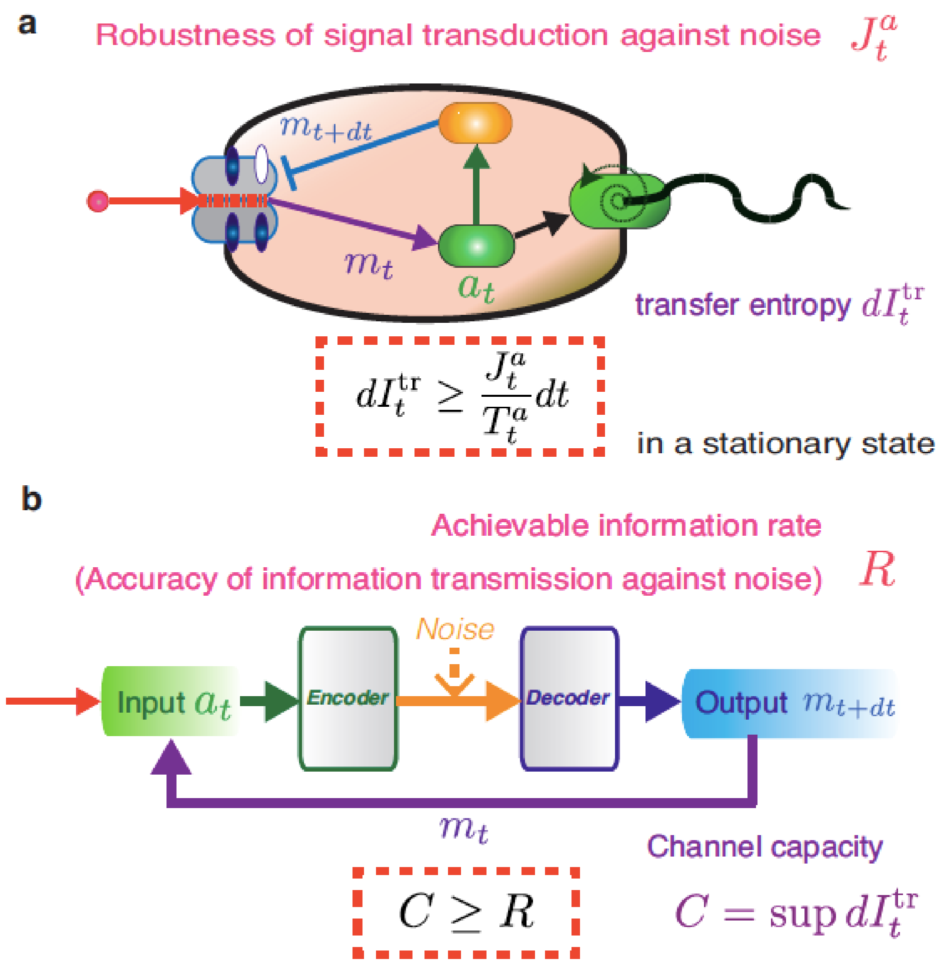
Red: robustness of adaptation

Green: information-thermodynamic bound Ξ_t^{info}

Blue: conventional thermodynamic bound Ξ_t^{SL}

- ✓ Information thermodynamics gives a stronger bound!
- ✓ The adaptation dynamics is inefficient (dissipative) as a conventional thermodynamic engine, but efficient as an information-thermodynamic engine.

Comparison with Shannon's Information Theory



Second law of information thermodynamics

Information $dI^{\mathrm{tr}}{}_t$
gives the bound of robustness $J^a{}_t$

Well-defined in living cells

Shannon's second theorem

Information (channel capacity) C
gives the bound of achievable rate R

How to define in living cells??

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- Fluctuation theorem for autonomous information processing

S. Ito & T. Sagawa, *Phys. Rev. Lett.* **111**, 180603 (2013).
Review: S. Ito & T. Sagawa, arXiv:1506.08519 (2015).
N. Shiraishi & T. Sagawa, *Phys. Rev. E* **91**, 012130 (2015).

- Information thermodynamics of biochemical signal transduction
  - ✓ Transfer entropy characterizes the **robustness** of adaptation

S. Ito & T. Sagawa, *Nature Communications* **6**, 7498 (2015).

Review of information thermodynamics:
J. M. R. Parrondo, J. M. Horowitz, & T. Sagawa, *Nature Physics* **11**, 131-139 (2015).

Thank you for your attention!