STOCHASTIC THERMODYNAMICS OF DISTRIBUTED SYSTEMS

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Consider a (perhaps time-varying) master equation:

$$\frac{dp_i(t)}{dt} = \sum_j K_{ij}(t) p_j(t)$$

- Example: Dynamics of a Turing Machine
- Example: (Noisy) dynamics of a digital gate in a circuit
- Example: (Noisy) dynamics of an entire digital circuit
- Example: Spike train going down an axon
- Example: Neuronal assemblies communicating

Consider a (perhaps time-varying) master equation:

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Just for fun,
let's see how Shannon entropy of p
evolves under this equation

Consider a (perhaps time-varying) master equation:

$$\frac{dp_i(t)}{dt} = \sum_j K_{ij}(t) p_j(t)$$

$$\frac{dS(p(t))}{dt} = \dot{Q}(t) + \dot{\Sigma}(t)$$

- $\dot{Q}(t) = \sum_{ij} K_{ij}(t) p_j(t) \ln \frac{K_{ji}(t)}{K_{ij}(t)}$ *Entropy flow rate*
- $\dot{\Sigma}(t) = \sum_{ij} K_{ij}(t) p_j(t) \ln \frac{K_{ij}(t) p_j(t)}{K_{ji}(t) p_i(t)}$ *Entropy production rate*

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- ***Entropy production (EP) rate is non-negative***

Van den Broeck and Esposito, *Physica A*, 2015

Consider a master equation that sends $p_0(x)$ to $p_1(x) = \sum_{x_0} P(x_1 \mid x_0)\, p_0(x)$

$$\frac{dp_i(t)}{dt} = \sum_j K_{ij}(t) p_j(t)$$

$$\frac{dS(p(t))}{dt} = \dot{Q}(t) + \dot{\Sigma}(t)$$

Integrate over time: $-\Delta Q = \Delta\Sigma - \Delta S$

- $\Delta S = S(p_1) - S(p_0)$ is gain in Shannon entropy of p
- $-\Delta Q$ is (Shannon) entropy flow from system between t = 0 and t = 1
- $\Delta\Sigma$ is total entropy production in system between t = 0 and t = 1
  - ***cannot be negative***

  (I.e., the second law of thermodynamics)

Van den Broeck and Esposito, *Physica A*, 2015

GENERALIZED LANDAUER BOUND

- System connected to multiple reservoirs, e.g., heat baths at different temperatures. (So "$k_B T$" not defined.)
- Arbitrary number of states
- Arbitrary initial distribution p_0
- Arbitrary dynamics $P(x_1 \mid x_0)$

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$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

Entropy Production ($\Delta\Sigma$) is non-negative. So:

"*Generalized Landauer's bound*":

Entropy flow (i.e., $-\Delta Q$) $\geq S(p_0) - S(p_1)$

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- Assume local detailed balance

Then: -ΔQ ***is (temperature-normalized) heat flow into environment***

EXAMPLE – LANDAUER'S CONCLUSION

- System evolves while connected to <u>*single*</u> heat bath at temperature *T*

  Then heat flow into environment $= -k_B T \, \Delta \boldsymbol{Q}$

- Two possible states
- p_0 uniform
- Process implements bit erasure (so p_1 a delta function)
- Assume local detailed balance

So generalized Landauer's bound says

$$\text{Total heat flow into environment} \geq k_B T \ln[2]$$

Landauer's conclusion

(Parrondo et al., *Nature Physics 2015*, Sagawa, *J. Stat. Mech. 2014*, Hasegawa et al., *Phys. Letters A 2010*, Wolpert, *Entropy 2015*, *etc.*)

IMPLICATATION OF GENERALIZED LANDAUER BOUND

$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

p_0 is initial distribution, i.e., distribution over inputs.

- *Fixed by environment / previous computations*.

p_1 is ending distribution, i.e., distribution over outputs.

- *Fixed by the (possibly noisy) computation, $P(x_1 \mid x_0)$*

Increasing noise in computation
(increases entropy of ending distribution and so)
reduces minimal thermodynamic cost

WHAT IS REALLY IMPORTANT THERMODYNAMICALLY?

$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

- System evolves while connected to *single* heat bath at temperature *T*

  Then heat flow into environment = $-k_B T \, \Delta \boldsymbol{Q}$

- At scale of real computers and brains, $k_B T [S(p_0) - S(p_1)]$ is small

- At scale of real computers and brains, $\Delta\Sigma$ **is dominant cost**

What determines $\Delta\Sigma$?

1) Given a fixed computer, varying distribution over inputs changes expected thermodynamic costs – how exactly?

In particular, *how does EP generated by a fixed process* $P(x_1 \mid x_0)$ *depend on the initial distribution,* $P(x_0)$?

Dependence of EP on initial distribution

- Arbitrary dynamics $P(x_1 \mid x_0)$
- ***Assume system is thermo. reversible for initial distribution q_0***

I.e., $\Delta\Sigma(q_0) = 0$

- Run that system with initial distribution $p_0 \neq q_0$ instead:

$$\Delta\Sigma(p_0) = D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1) \geq 0$$

where D(. || .) is relative entropy (KL divergence)

Wolpert, D., Kolchinsky, A., *New J. Phys.* (2020)
Riechers, P.. Gu, M., *Phys. Rev. E* (2021)
Kolchinsky, A., Wolpert D., *arxiv:2103.05734*

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Any nontrivial process that is thermodynamically reversible for one initial distribution will not be for any other initial distribution

Example/

- ***Two*** distinct bit-erasing gates, each with thermo. rev. initial distribution q_0
- Run gates in parallel, on bits x^A and x^B, with initial distribution $p_0(x^A, x^B)$
- Assume $p_0(x^A) = q_0(x^A)$ and $p_0(x^B) = q_0(x^B)$.

- So each gate, by itself, generates zero EP. But:

If $p_0(x^A, x^B)$ statistically couples the bits, then
full system is **not** *thermo. reversible,*
and generates nonzero EP

- **Formally**: Since gates are distinct, the thermo. rev. *joint* distribution is

$q_0(x^A, x^B) = q_0(x^A)q_0(x^B)$.

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- **Formally**: Since gates are distinct, the thermo. rev. *joint* distribution is $q_0(x^A, x^B) = q_0(x^A)q_0(x^B)$. So $D(p_0 \,||\, q_0) - D(p_1 \,||\, q_1) \neq 0$

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- Intuition: **Running two thermo. reversible gates in parallel loses information in their initial coupling, and so is not thermo. reversible**.

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- **Broader lesson**: ***Modularity increases EP***

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- **Broader lesson**: Whatever its benefits might be,

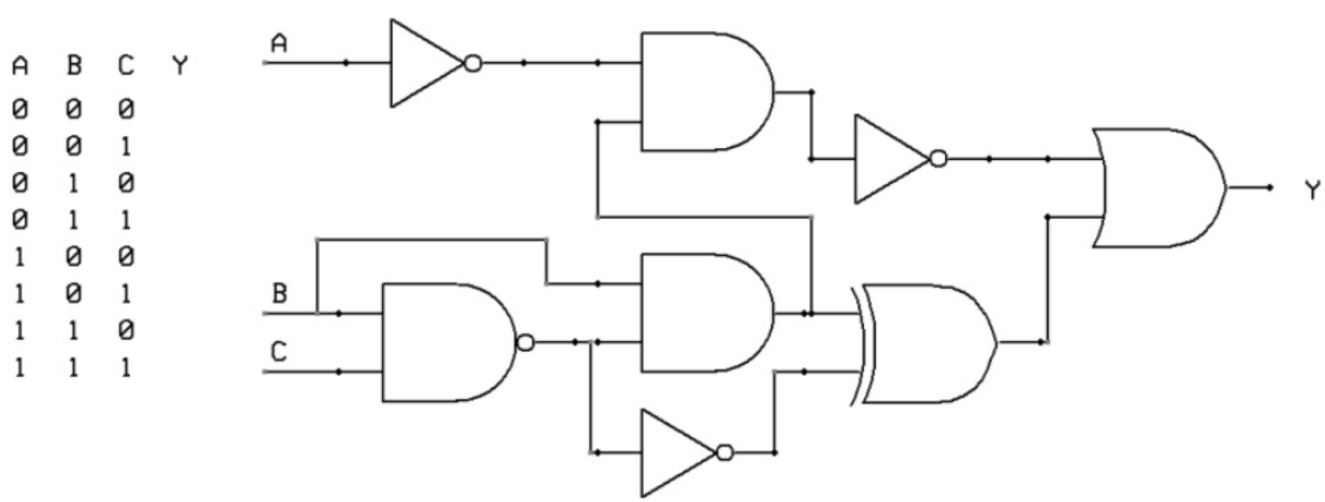
  modularity is thermodynamically costly (!)

Example - Thermodynamics of circuits

- Currently, all mass-produced computers are implemented with circuits.
- The simplest circuit is one without loops or branches (a "straight-line program")
- If set of allowed gates are a universal basis (e.g., NAND gates), then can build a circuit with them to implement any desired Boolean function.

$$-\Delta Q = \Delta\Sigma + S(p_0) - S(p_1)$$

- For fixed $P(x_1 \mid x_0)$, changing p_0 changes $S(p_0) - S(p_1)$
- N.b., the same $P(x_1 \mid x_0)$ - e.g., same AND gate - has different p_0, depending on where it is in a circuit.
- So *even for a thermo. reversible gate* ($\Delta\Sigma(p_0) = 0$), ***changing the gate's location in a circuit*** (changes $S(p_0) - S(p_1)$ and so) ***changes*** $-\Delta Q(p_0)$



- Changing a gate's location in a circuit changes $S(p_0) - S(p_1)$, and so changes the heat it produces, $-\Delta Q(p_0)$

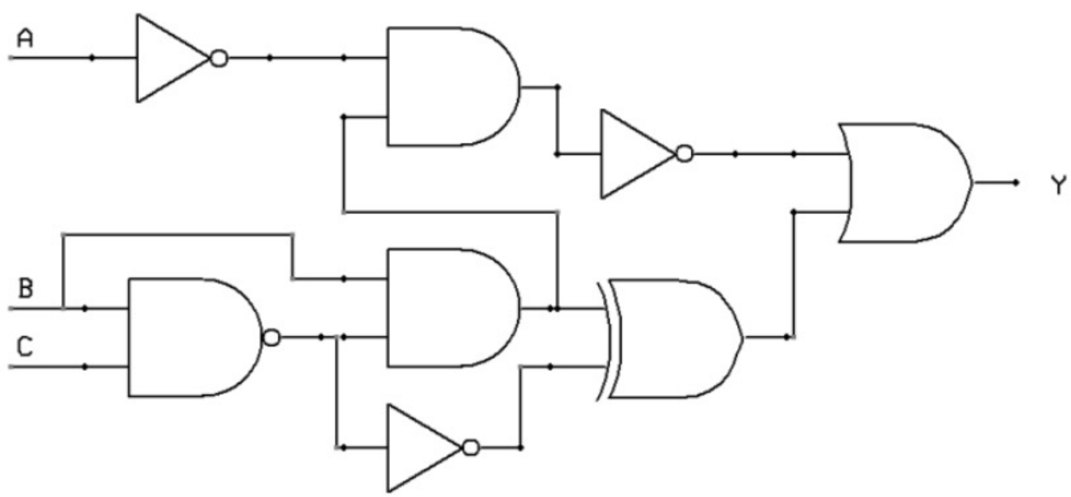
- Sum those heats over all gates to get minimal heat flow of that circuit

> Different circuits implementing *same* Boolean function on *same* input distribution have *different* minimal heat

- Formally, those differences in minimal heat of the circuits are differences in EPs of the circuits, arising due to modularity of gates

  ➢ A new circuit design optimization problem

A	B	C	Y
0	0	0	
0	0	1	
0	1	0	
0	1	1	
1	0	0	
1	0	1	
1	1	0	
1	1	1	



NOTATION:

$$I\big(P(X_1, X_2, \ldots)\big) = \left[\sum_i S(P(X_i))\right] - S(P(X_1, X_2, \ldots))$$

- "Multi-information" (also called "total correlation")

- A generalization of mutual information

- Quantifies how much information is shared among the X_i

WHAT CIRCUIT TO COMPUTE A GIVEN FUNCTION f?

(Partial) answer: Assume each gate re-initializes the upstream gates that provided its input.

Then change in total Landauer cost if use circuit C′ rather than C to compute f:

$$\sum_{g \in C'} I(p^{pa(g)}) - \sum_{g \in C} I(p^{pa(g)})$$

where g indexes gates.

I.e., choose circuit that implements f with ***smallest sum of multi-informations*** of input distributions into its gates.

Wolpert, D., Kolchinsky, A.,*New J. Physics* (2020)

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A *global* circuit design optimization problem.

Wolpert, D., Kolchinsky, A., *New J. Physics* (2020)

FLUCTUATION THEOREMS

At the macroscopic scale, expected entropy cannot decrease;

Can <u>always</u> tell if a movie of a macroscopic process runs backward

At the microscopic scale, expected entropy cannot change;

Can <u>never</u> tell if a movie of a microscopic process runs backward

---

What happens at mesoscopic scale?

FLUCTUATION THEOREMS

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- $$\dot{\Sigma} = \sum_{ij} K_{ij} p_j(t) \ln\left[\frac{K_{ij} p_j(t)}{K_{ji} p_i(t)}\right]$$

These are <u>expectations over trajectories</u>.

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These are expectations over trajectories.
Can also define trajectory-level thermodynamic quantities:

- Stochastic entropy if system in state i at time t: $s_i(t) = -\ln p_i(t)$
- Expectation of stochastic entropy is Shannon entropy, S(p(t))

FLUCTUATION THEOREMS

Can define trajectory-level thermodynamic quantities.

- Stochastic entropy if system in state i at time t: $s_i(t) = -\ln p_i(t)$

***Integral fluctuation theorem (FT)** constrains the average over trajectories of total (time-integrated) EP along a trajectory:*

$$\langle e^{-kT\sigma} \rangle = 1$$

(Seifert, Reports on Progress in Physics, 2012)

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Integral fluctuation theorem (FT) constrains the average over trajectories of total (time-integrated) EP along a trajectory:

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- ***Apply Jensen's inequality: expected EP over trajectories is non-negative – second law, as before.***
- ***But nonzero probability that in any single trajectory, EP < 0***

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- ***But nonzero probability that in any single trajectory, EP < 0***

- Quantifies probability that at any scale, movie runs backward

THERMODYNAMIC UNCERTAINTY RELATIONS (TURs)

- ***x*** is a *trajectory* of system states during a given time interval

- A *current* $J(\boldsymbol{x})$ is any (!) function of the state transitions in ***x*** that is odd under time-reversal

  Examples: Net charge flow from anode to diode;
  Net number of times a particular neuron fires;
  Net value of predictive coding error signals.

- In many conditions (e.g., a steady state) a *Thermodynamic Uncertainty Relation* bounds current statistical precision by $\Delta\Sigma$:

$$\frac{\Delta\Sigma}{2k_B} \geq \frac{\langle J\rangle^2}{Var(J)}$$

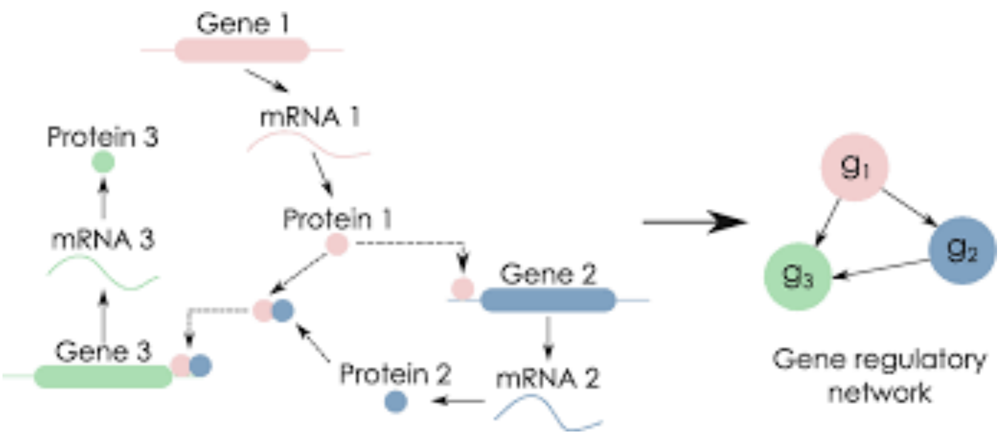
- ***Example***: If variance in predictive coding error signals is small, then small expected errors is *necessary* for small thermodynamic cost

Accurate predictions in predictive coding is necessary to have low energetic cost

THERMODYNAMICS OF CO-EVOLVING COMPUTERS

- Many examples of multiple asynchronous co-evolving computers
  - organelles in a cell
  - neurons in a brain
  - organs in a biological organism
  - humans in a social organization

- Network topology of interactions has major thermodynamic consequences

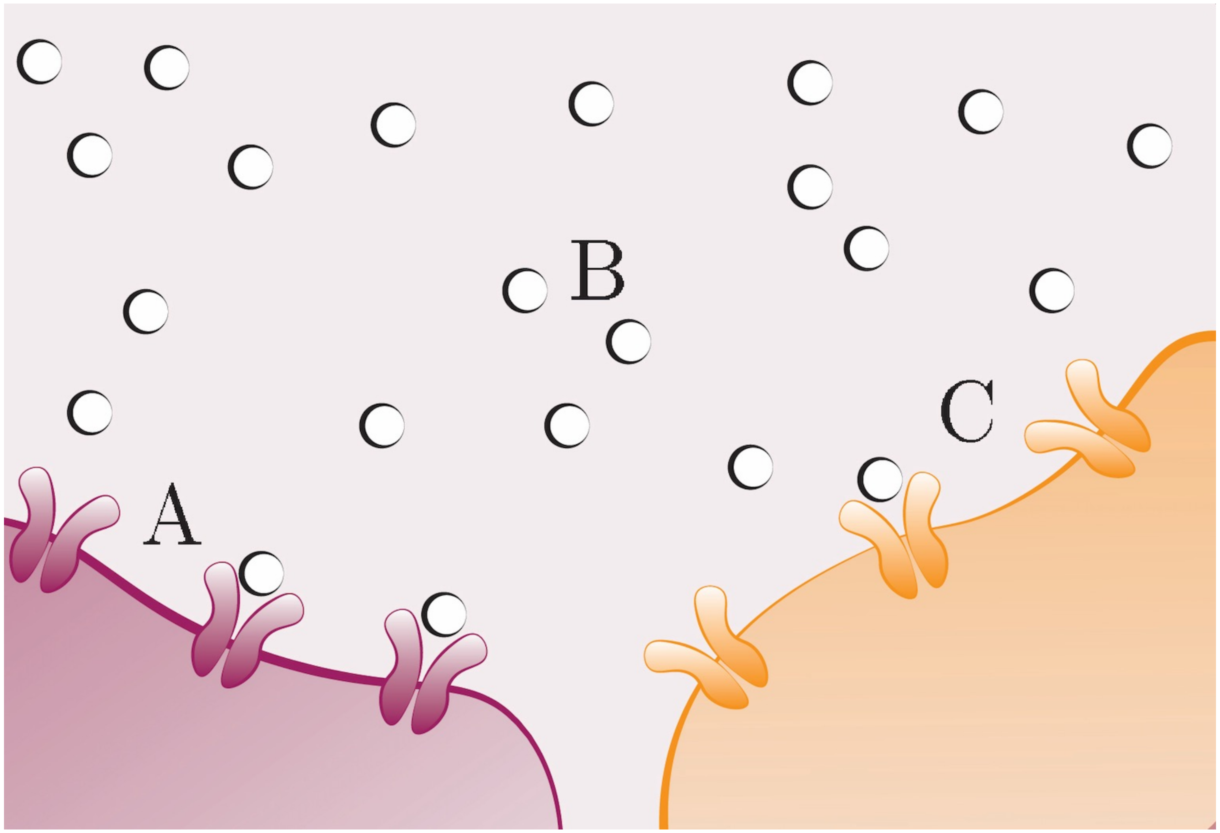


Much of conventional stochastic thermodynamics

– including (almost) all FTs and TURs –

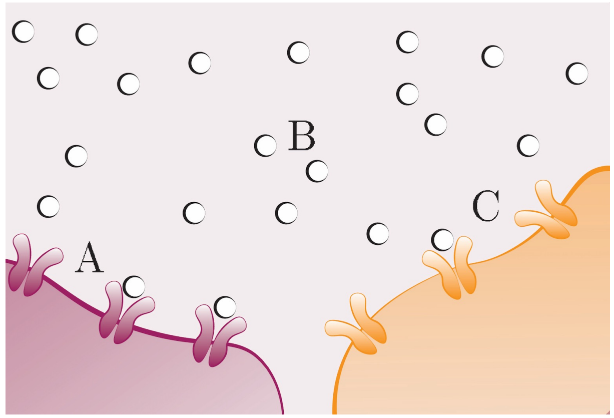
is formulated for single systems, ***not*** multiple interacting systems

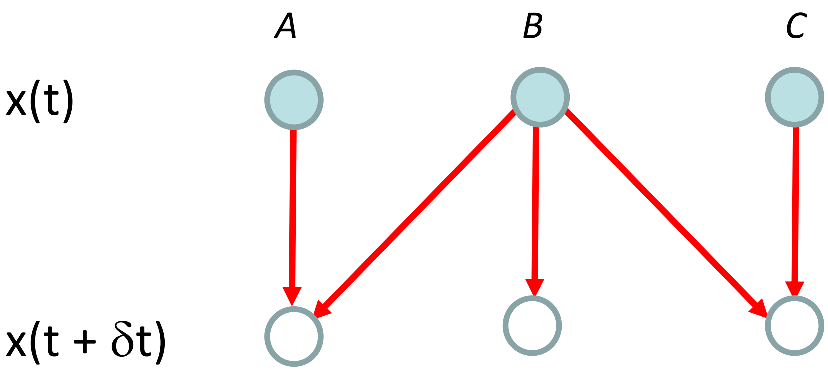
Example of interacting systems



- B is level of ligand concentration in medium
- A is cell wall detectors of ligand concentration
- C is cell wall detectors of ligand concentration

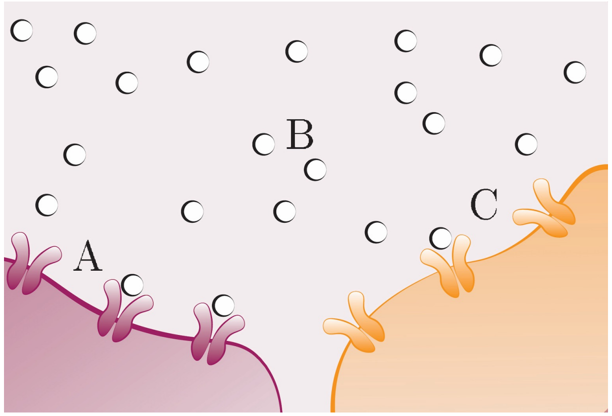
Example of interacting systems

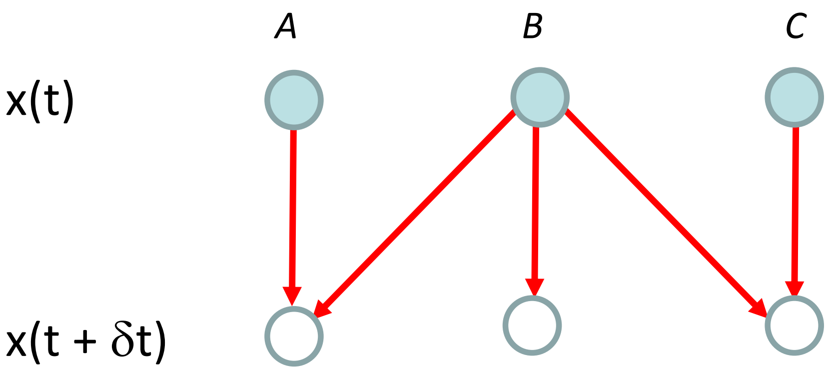




- Red arrows indicate dependencies of rate matrices of the three systems
- N.b., {B} evolves independently, but is observed by {A} and {C}
- {A} and {C} not *physically* coupled, but become *statistically* coupled with time

Example of interacting systems

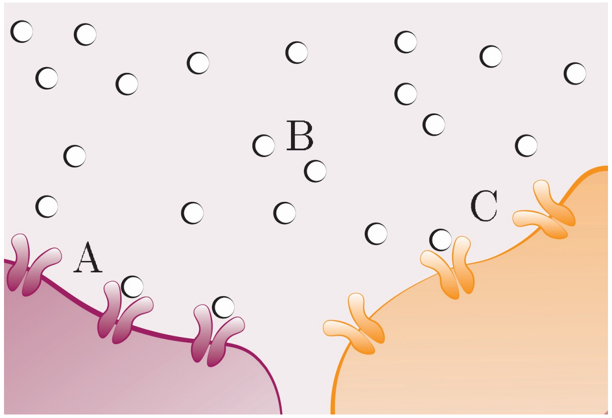


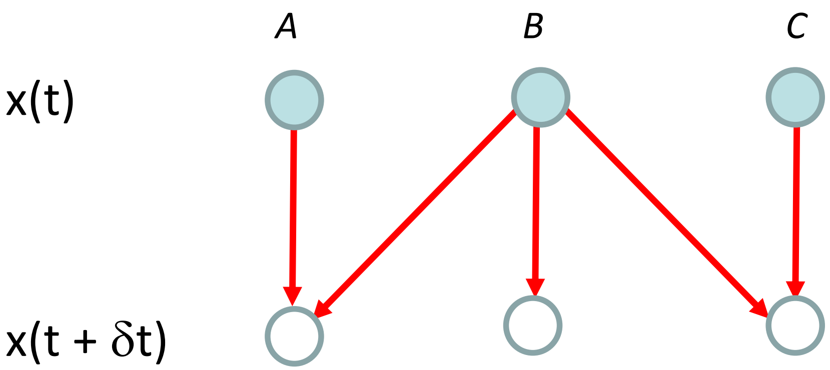


A *unit* *r* is a set of systems that evolve autonomously

- {AB}, {B}, and {BC} are units

Example of interacting systems

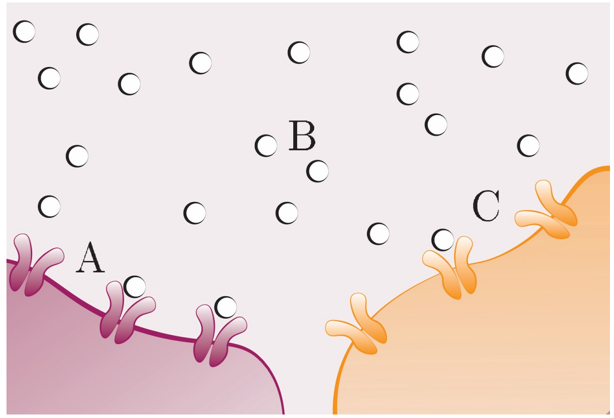


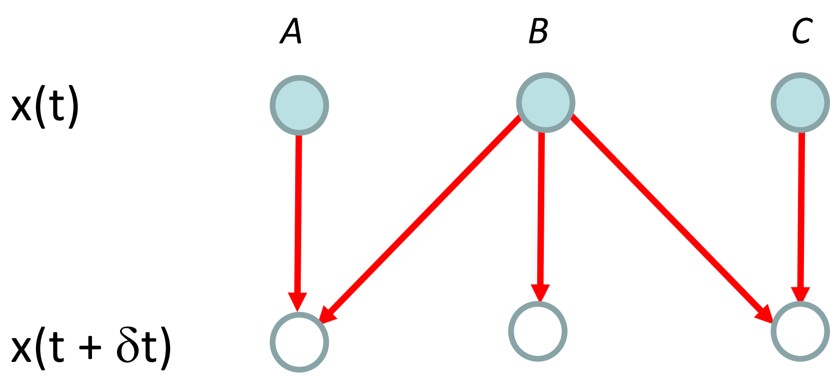


A *unit* *r* is a set of systems that evolve autonomously

- Each unit has its own master equation, its own EP, own FTs, own TURs, etc.

Example of interacting systems





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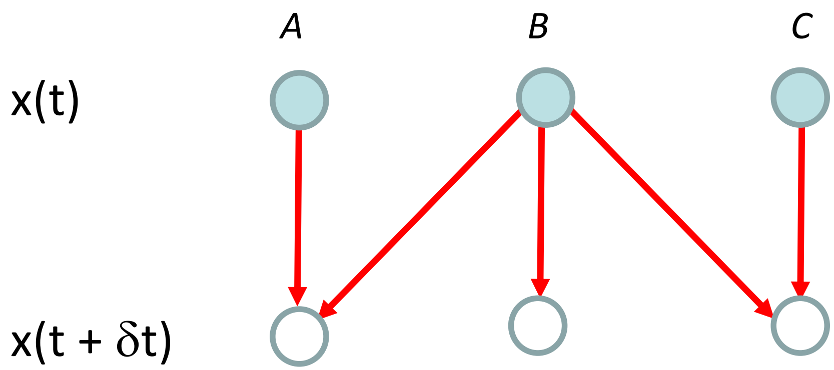
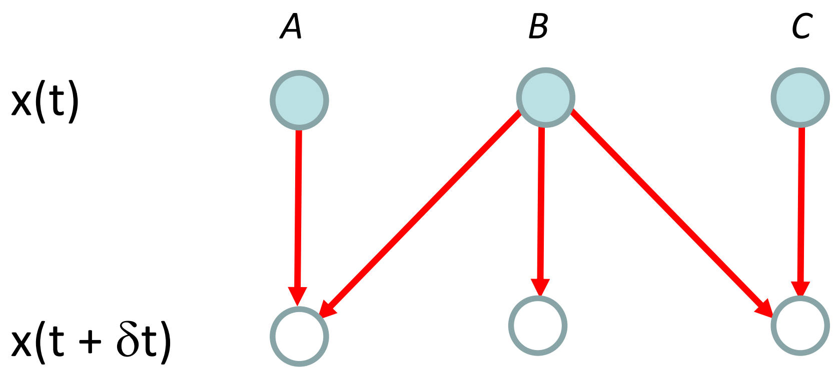
How are fluctuations in EPs of the units coupled?



- *Conditional* integral fluctuation theorem: For any unit r,

$$\langle e^{\sigma^r - \sigma} | \sigma^r \rangle = 1$$



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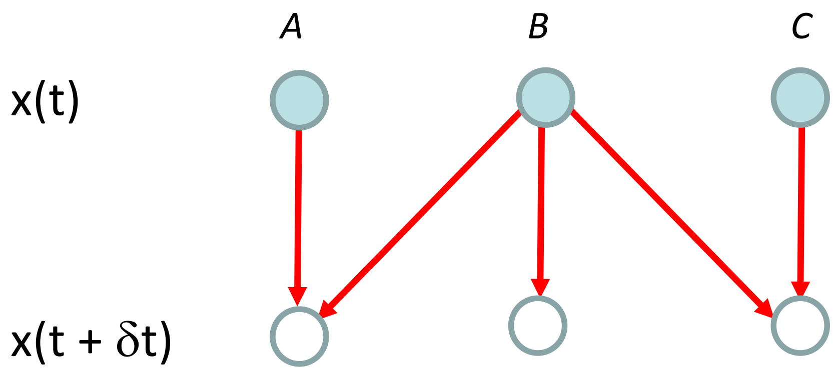
- System-wide EP for trajectory **x**: $\sigma(\mathbf{x}) = \widehat{\sum_{r'}} \sigma^{r'}(\mathbf{x}) - \Delta I^*(\mathbf{x})$
  - $\widehat{\Sigma}_{r'} \sigma^{r'}(\mathbf{x})$ is "inclusion-exclusion sum", of unit EPs over trajectory **x**
  - $\Delta I^*(\mathbf{x})$ is (change in) "inclusion-exclusion sum" of Shannon entropies



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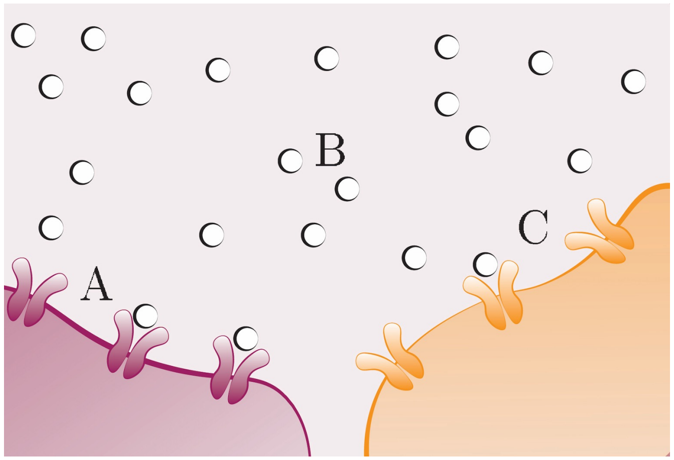
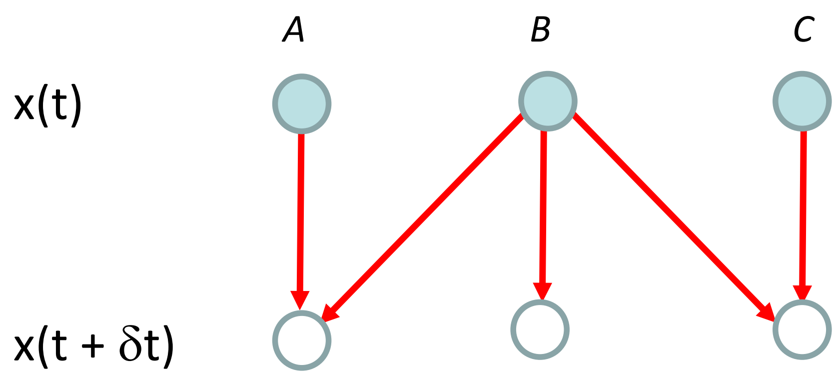
Combining: For *any* unit r, $\widehat{\sum_{r'}} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^* \rangle \geq \langle \sigma^r \rangle$

Speed limit theorem for interacting systems





$$\widehat{\sum}_{r'} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^{*} \rangle \geq \langle \sigma^{r} \rangle$$

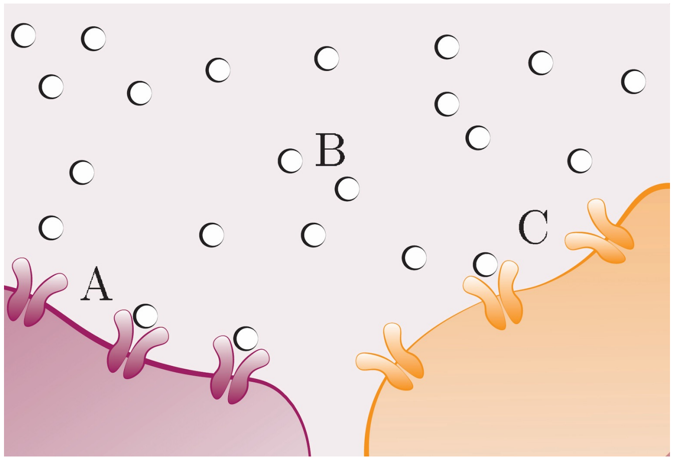
- Using this result repeatedly for different choices of unit *r* gives:

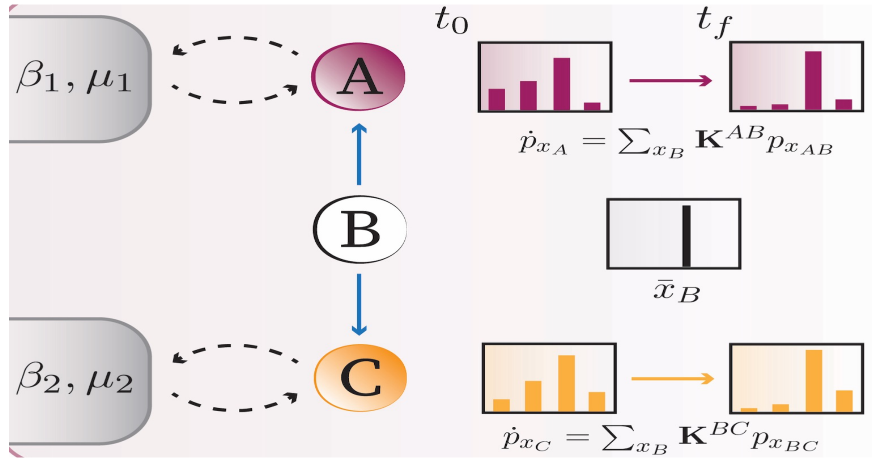
$$\min\left[\left\langle \sigma^{BC} \right\rangle, \left\langle \sigma^{AB} \right\rangle\right] - \left\langle \sigma^{B} \right\rangle \geq \Delta I(A;C\,|\,B)$$

where $I(A\,;\,C\mid B)(t)$ is mutual information between the two types of receptor, conditioned on ligand concentration level

- So if want to change conditional mutual information a lot during fixed time interval, must pay for it with large EP of both the units BC and AC

Strengthened second law for interacting systems





$$\widehat{\sum_{r'}} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^* \rangle \geq \langle \sigma^r \rangle$$

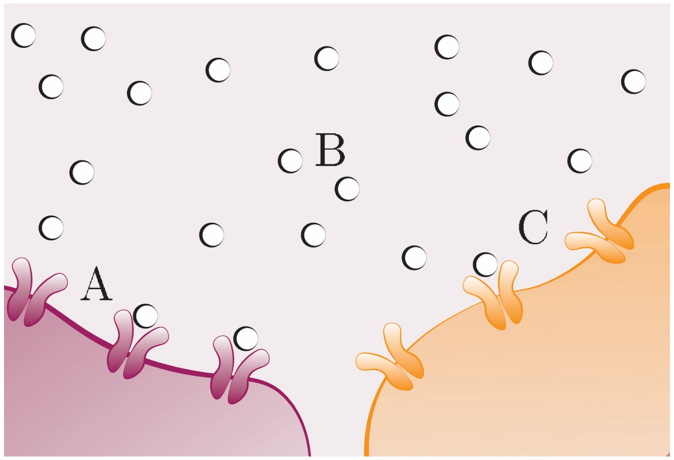
- If ligand concentration is constant in time, *total* EP of full system is bounded by

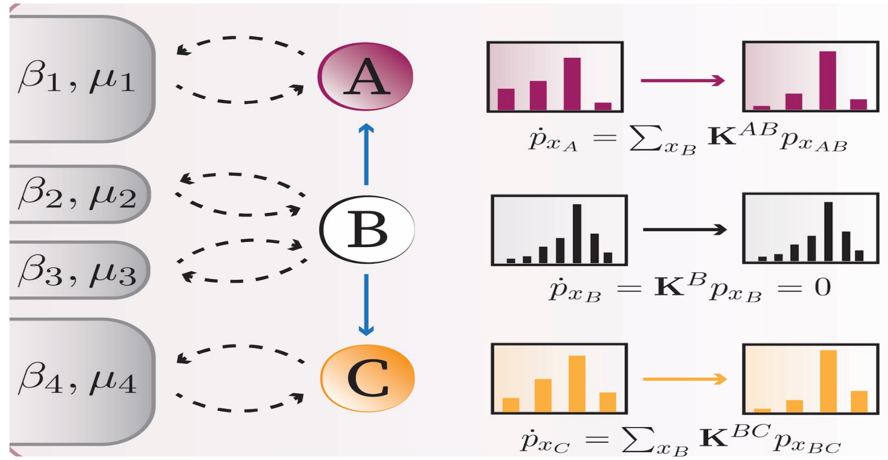
$$\langle \sigma \rangle \geq -\Delta I(A;C \,|\, B) \geq 0$$

- A larger lower bound on total EP of full system than the second law,

  reflecting informational coupling among ligand concentration and two receptor types

New *kind* of TUR





$$\widehat{\sum}_{r'} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^* \rangle \geq \langle \sigma^r \rangle$$

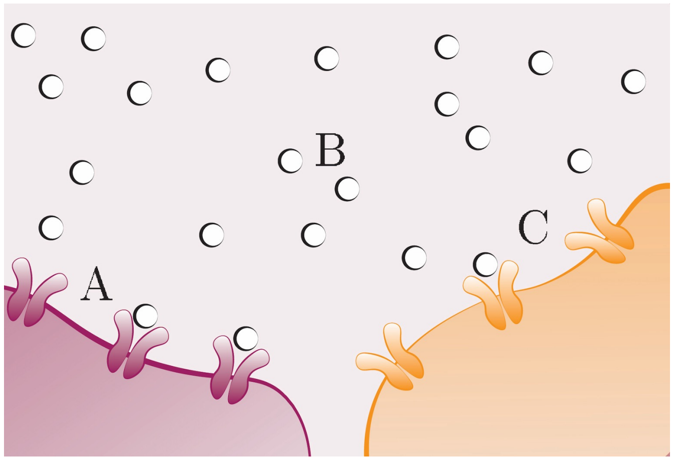
- Suppose ligand concentration in stationary state, so standard TUR applies to that system, *but overall system does not obey conditions for any conventional TUR*.

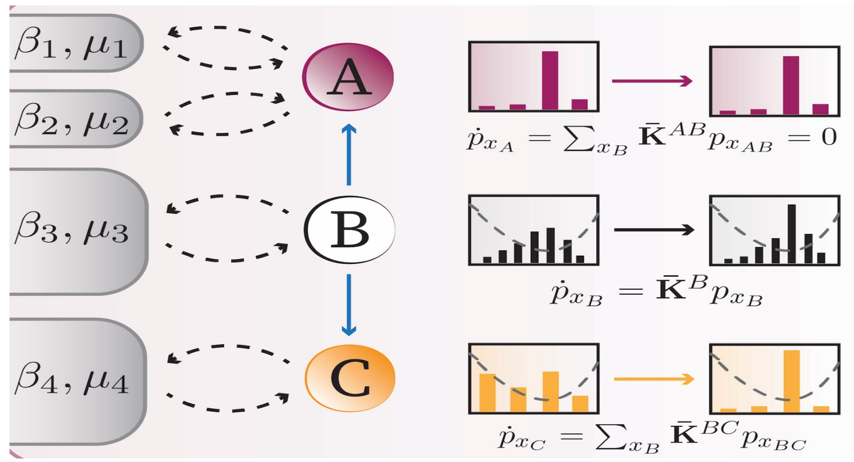
- <u>So conventional TUR does not apply to overall system</u>

- Even so: $\langle \sigma \rangle \geq \frac{2k \langle J_B \rangle^2}{\mathrm{Var}(J_B)} + \max\left[\Delta I(A;C \mid B), 0\right]$

- So if ligand concentration varies in a noisy cyclic process, and is in a stationary state, then the less noise in the cycling, the more EP is produced by full system

Strengthened second law for interacting systems





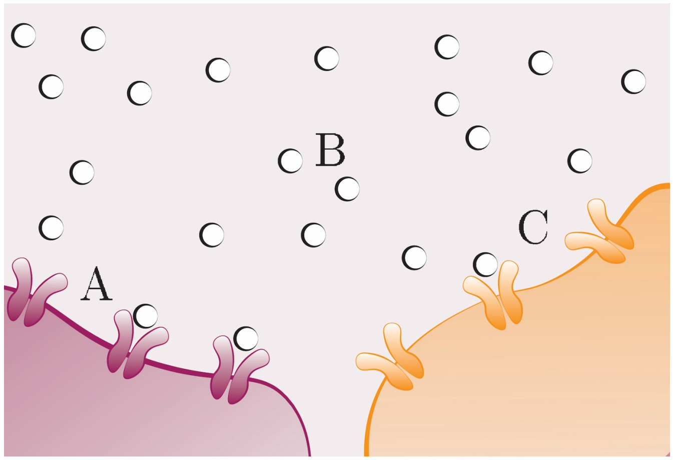
$$\widehat{\sum_{r'}} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^{*} \rangle \geq \langle \sigma^{r} \rangle$$

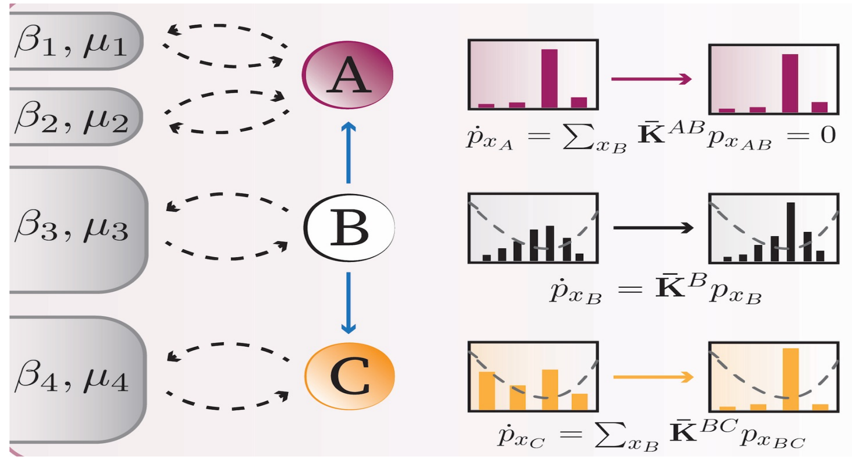
- Suppose all rate matrices constant in time (no mechanical work), and first receptor is in a stationary state:

$$\langle \sigma \rangle \geq \left\langle \sigma^{AB} \right\rangle + \left\langle \sigma^{BC} \right\rangle$$

- A larger lower bound on total EP of full system than the second law, reflecting structure of interactions among the three systems

New *kind* of TUR





$$\widehat{\sum_{r'}} \left\langle \sigma^{r'} \right\rangle - \langle \Delta I^* \rangle \geq \langle \sigma^r \rangle$$

- Suppose that in addition, ligand concentration starts in equilibrium. Then joint system AB would be in stationary state. However, joint system BC is relaxing to equilibrium.

- Systems AB and BC obey *different* TURs, and no conventional TUR applies to full system

- Even so: $\langle \sigma \rangle \geq \dfrac{2k\langle J_{AB}\rangle^2}{\mathrm{Var}(J_{AB})} + \dfrac{2[\tau \, j_{BC}(\tau)]^2}{\mathrm{Var}(J_{BC}(\tau))}$

CONCLUSIONS

- Exact equations for entire entropy flow of a system:

$$EF(p_0) = \text{Landauer cost } (p_0) + EP(p_0)$$

- Thermodynamic Kolmogorov complexity is bounded (unlike conventional Kolmogorov complexity)
- Average work to run a TM is infinite
- Different circuits, all implementing the same function, all using thermodynamically reversible gates, have different thermodynamic costs.
- Very difficult problems of finding least-cost circuit for a given function.
- For real digital computers, brains, etc., dominant cost is $EP(p_0)$, not Landauer cost
- TURs, speed limit theorems, mismatch cost, all provide lower bounds on $EP(p_0)$ arising from how a computer is used and how it performs.

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