THERMODYNAMICS OF MULTIPARTITE PROCESSES WITH CONSTRAINTS ON RATE MATRIX DEPENDENCIES

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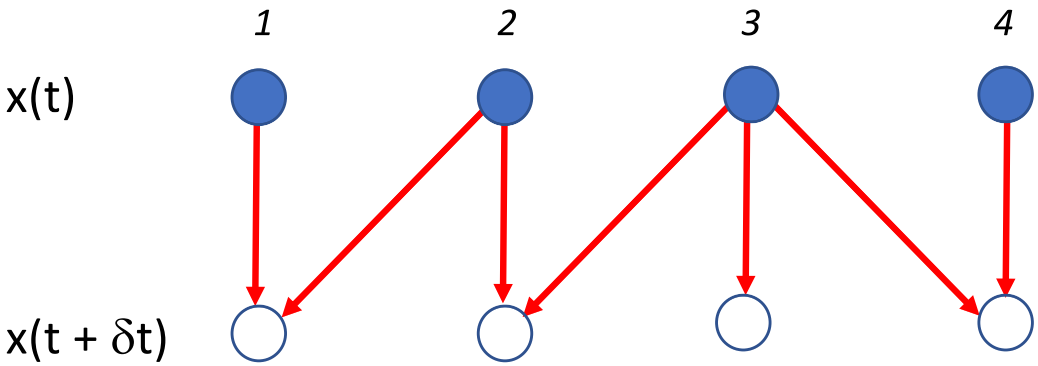
Example of a multipartite process



- Four subsystems, {1, 2, 3, 4}
- Red arrows indicate the dependencies of their rate matrices
- N.b., {3} evolves independently, but is observed by {2} and {4}
- So {2} and {4} are not physically coupled, but become statistically coupled with time

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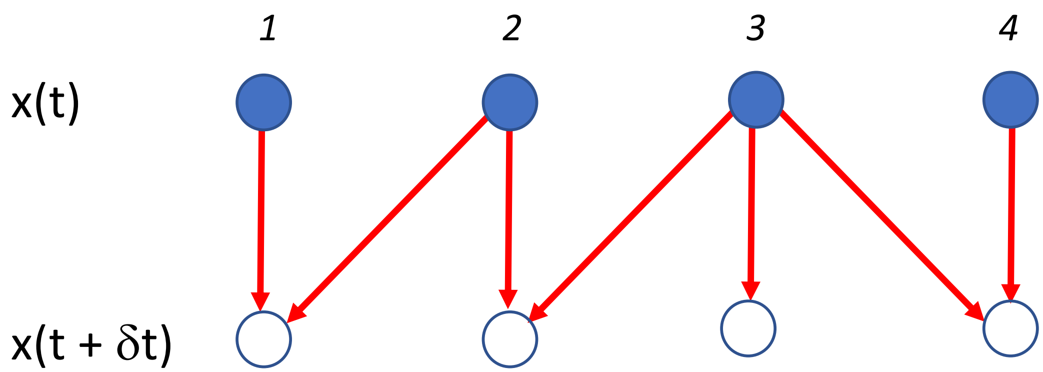

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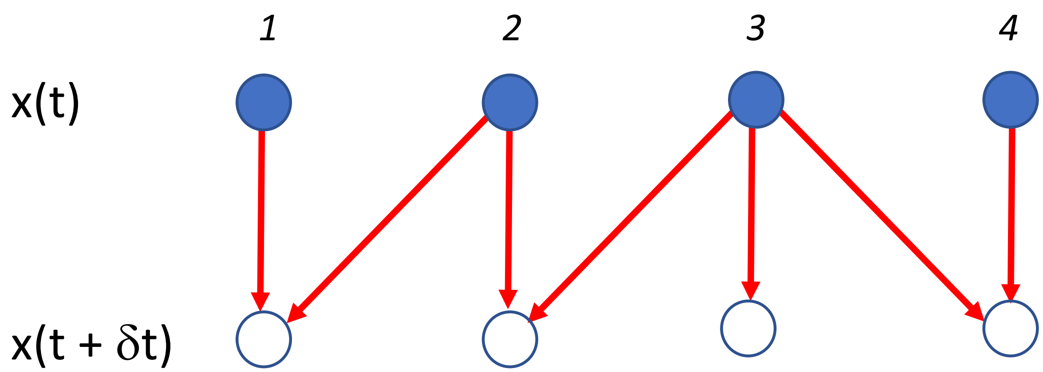
How does minimal entropy production (EP) rate depend on red arrow graph?
How are EP fluctuations of the subsystems coupled?

This talk



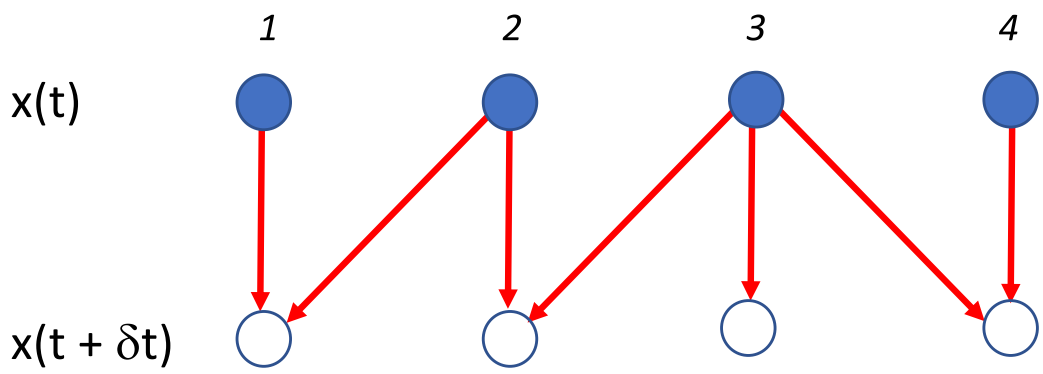
1) **Trajectory-level thermodynamics of multipartite processes**

2) First decomposition of system-wide EP in terms of subsystem properties and an information-theoretic property of “red arrow graph”

3) Resultant lower bounds on expected EP rate in terms of red arrow graph

4) Second decomposition of system-wide EP in terms of subsystem properties and an information-theoretic property of “red arrow graph”

5) Resultant “vector” fluctuation theorem in terms of red arrow graph

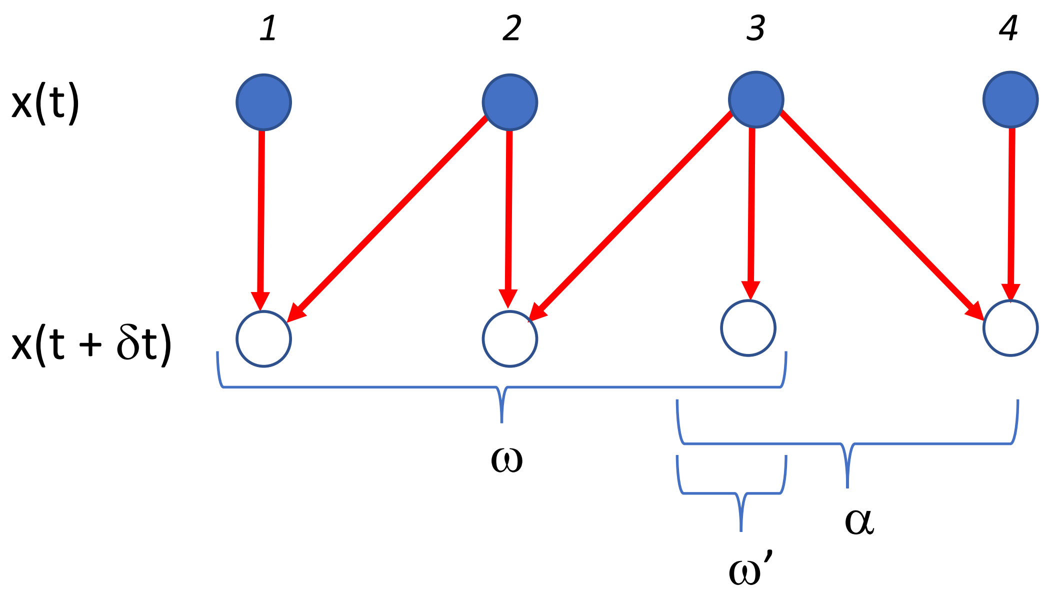


N – *set of subsystems*
x – *joint state of all subsystems*
$x_i(t)$ – *state of subsystem i at time t*

Since it's a multipartite process:

$$\frac{dp_x(t)}{dt} = \sum_{x'} \sum_{i \in N} K_x^{x'}(i;t) p_{x'}(t)$$

$$\forall x, x' : x_{-i} \neq x'_{-i}, K_x^{x'}(i;t) = 0$$

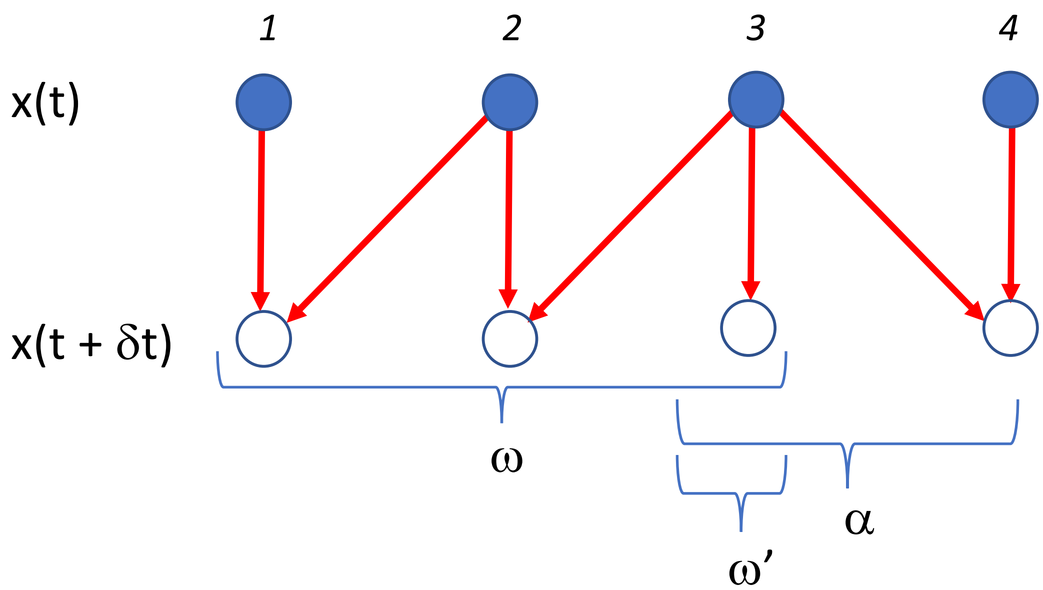


$$\frac{dp_x(t)}{dt} = \sum_{x'} \sum_{i \in N} K_x^{x'}(i;t) p_{x'}(t)$$

- A ***community*** r is a set of subsystems such that for every $i \in r$, $K(i;t)$ depends only on other subsystems $j \in r$:

$$K_x^{x'}(i;t) = K_{x_r}^{x'_r}(i;t)\delta(x'_{-r}, x_{-r})$$

- Dynamics of $\mathbf{x}_r$ depends only on $\mathbf{x}_r$; communities are "self-contained"



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$$K_x^{x'}(i;t) = K_{x_r}^{x'_r}(i;t)\delta(x'_{-r}, x_{-r})$$

- A ***community structure*** is a set of communities, closed under intersection, that covers N

Subsystem local detailed balance (SLDB)

Each subsystem is in contact with its own heat reservoirs:

$$\frac{K^{x'_r}_{x_r}(i;k,t)}{K^{x_r}_{x'_r}(i;k,t)} = \beta^k_i \left[H_{x'_r}(i;t) - H_{x_r}(i;t)\right]$$

for all i, k, t where

- r is a community containing subsystem i
- k is a heat reservoir
- $H_{x_r}(i;t)$ is ***local Hamiltonian*** of subsystem i

(Can be extended to include particle reservoirs)

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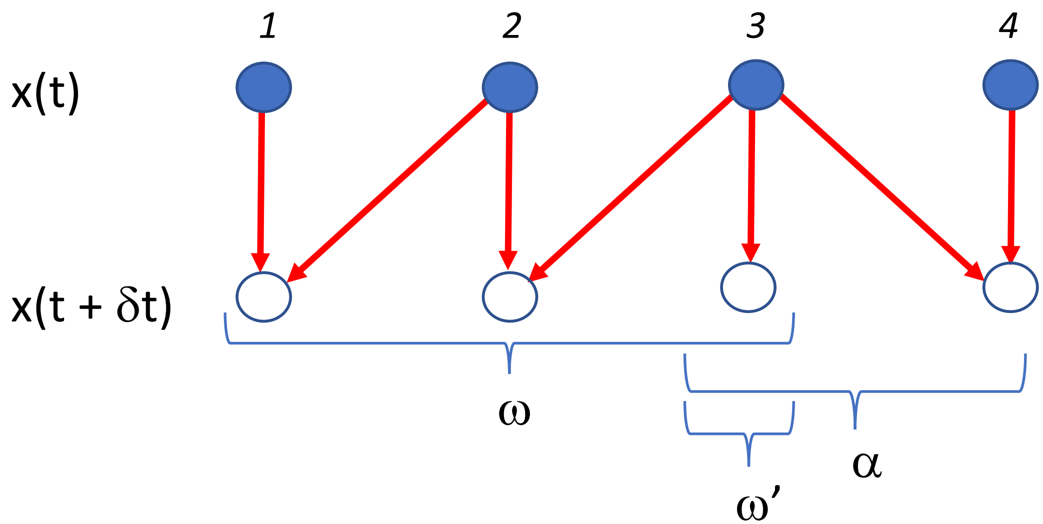
(Can be extended to include particle reservoirs)

- Therefore ***local heat flow*** into subsystem i during trajectory $\mathbf{x}$ is

$$Q^i(\mathbf{x}) = \sum_{\mathbf{j}} \beta_{\mathbf{i}}^{\mathbf{k(j)}} \left[\mathbf{H}_{\mathbf{x_r}(\tau(\mathbf{j}))}(\mathbf{i};\tau(\mathbf{j})) - \mathbf{H}_{\mathbf{x_r}(\tau(\mathbf{j-1}))}(\mathbf{i};\tau(\mathbf{j}))\right]$$

where $\mathbf{x}_r(\tau(\mathrm{j}))$ is community r's state at j'th time that subsystem i changes state

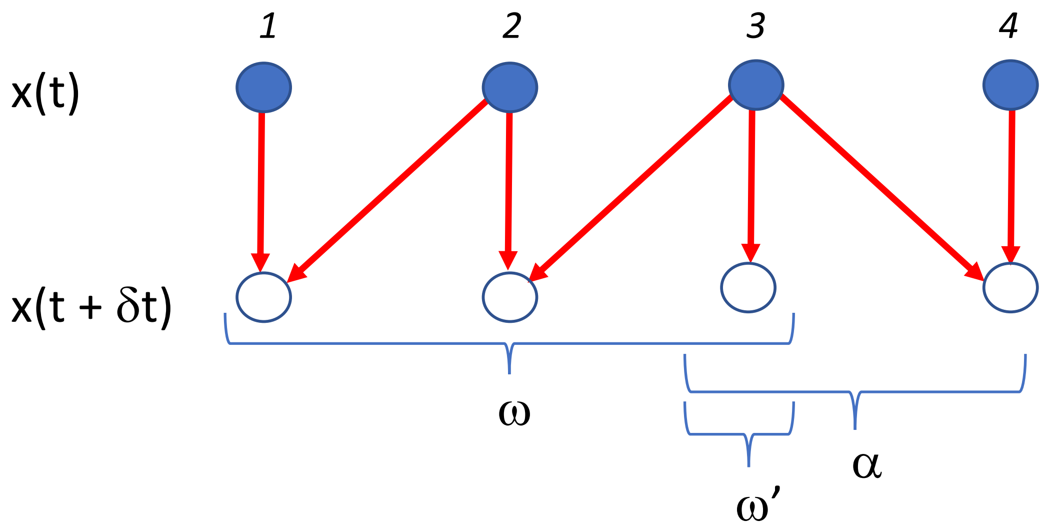


$$Q^i(\mathbf{x}) = \sum_{\mathbf{j}} \beta_{\mathbf{i}}^{\mathbf{k(j)}} \left[\mathbf{H}_{\mathbf{x_r}(\tau(\mathbf{j}))}(\mathbf{i};\tau(\mathbf{j})) - \mathbf{H}_{\mathbf{x_r}(\tau(\mathbf{j-1}))}(\mathbf{i};\tau(\mathbf{j}))\right]$$

- ***Local heat flow*** into community *r* during trajectory **x** is

$$Q^r(\mathbf{x}) = \sum_{i\in r} Q^i(\mathbf{x}_r)$$

- N.b., heat flow into community *r* only depends on states of subsystems in *r*



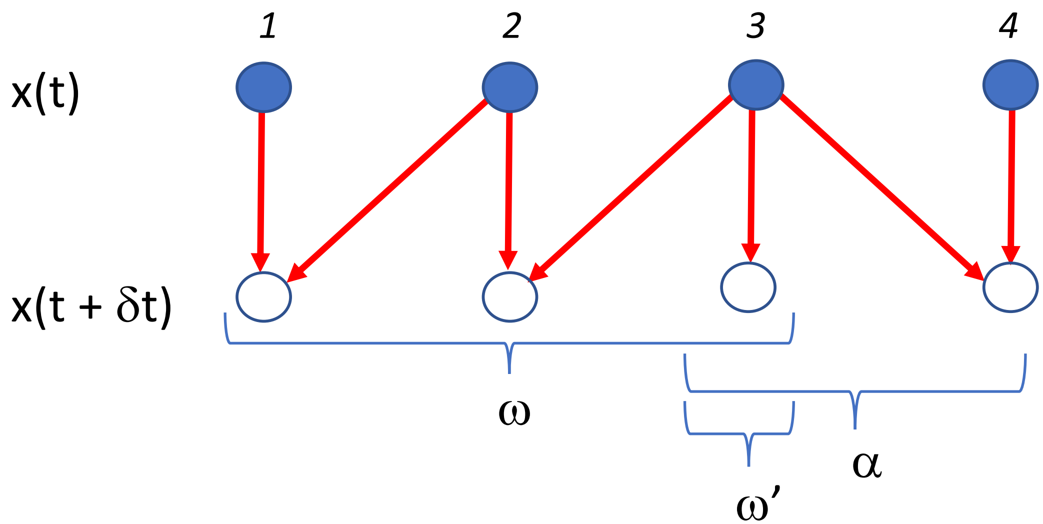
$$Q^r(\mathbf{x}) = \sum_{i \in r} Q^i(\mathbf{x}_r)$$

- ***Local EP*** of community r during trajectory $\mathbf{x}$ is

$$\sigma^r(\mathbf{x}_r) = \Delta s^r(\mathbf{x}_r) - Q^r(\mathbf{x}_r)$$

- where as usual the ***stochastic entropy*** of community r during trajectory $\mathbf{x}$ at time t is

$$s^r(\mathbf{x}_r(t)) = -\ln p_{\mathbf{x}_r(t)}(t)$$



- Let $R = \{r, r', \ldots\}$ be a set of communities (not necessarily a full community structure)

- Define

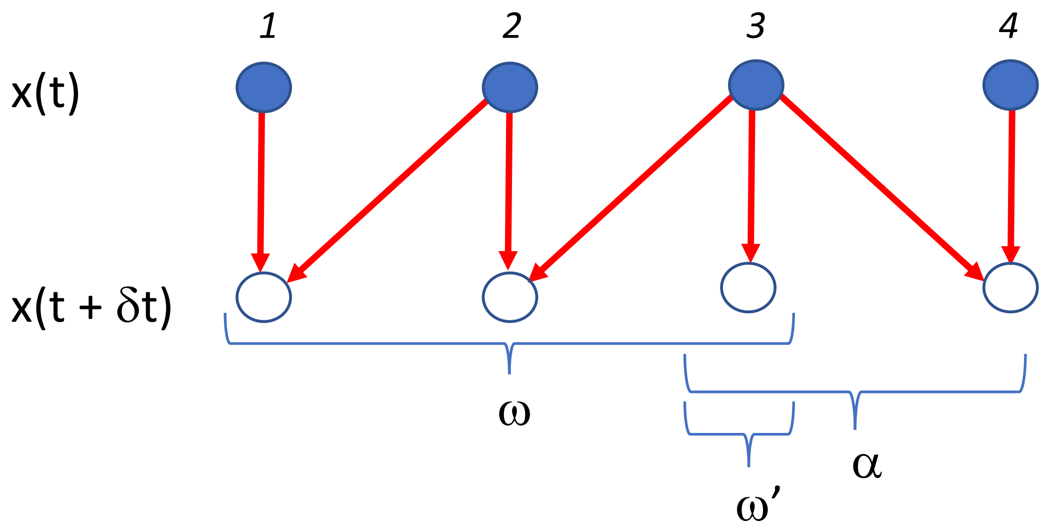
$$\vec{\sigma}^R(\mathbf{x}) = \Big(\sigma^r(\mathbf{x}), \sigma^{r'}(\mathbf{x}), \ldots\Big)$$

$$\sigma^{\cup R}(\mathbf{x}) = \Delta s(\mathbf{x}_{r \cup r' \cup \ldots}) - Q(\mathbf{x}_{r \cup r' \cup \ldots})$$

- ***"Vector-valued detailed fluctuation theorem"*** (DFT):

$$\ln\left[\frac{\mathbf{P}(\vec{\sigma}^R)}{\tilde{\mathbf{P}}(-\vec{\sigma}^R)}\right] = \sigma^{\cup R}(\mathbf{x})$$

(with usual definition of $\tilde{\mathbf{P}}(-\vec{\sigma}^R)$ as probability under a reverse protocol)



- Let $R = \{r, r', \ldots\}$ be a set of communities (not necessarily a full community structure)

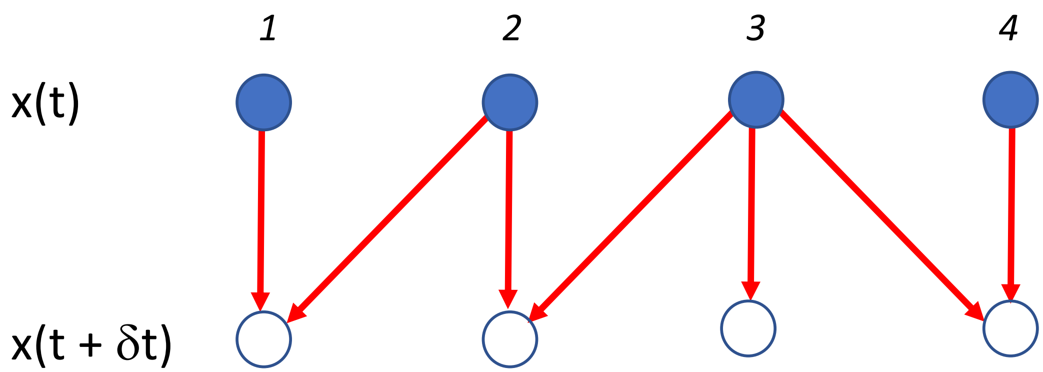
$$\ln\left[\frac{\mathbf{P}(\vec{\sigma}^R)}{\tilde{\mathbf{P}}(-\vec{\sigma}^R)}\right] = \sigma^{\cup R}(\mathbf{x})$$

- Subtract this DFT evaluated where R is a single community, r, from this DFT evaluated where R is a full community structure, to get a ***conditional IFT*****:**

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

where as before, σ is system-wide EP, and σ^r is EP of community r

This talk



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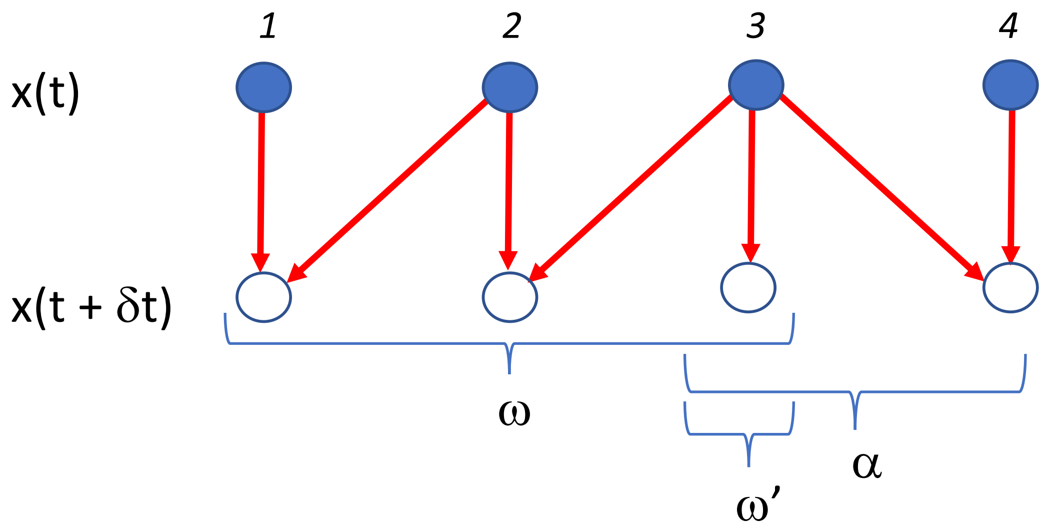

- For *any* community r, ***system-wide EP*** during trajectory $\mathbf{x}$ is

$$\sigma(\mathbf{x}) = \sigma^r(\mathbf{x}) + \Delta s^{X_{-r}|X_r}(\mathbf{x}) - Q^{-r}(\mathbf{x})$$

where

- as before, local EP $\sigma^r(\mathbf{x}_r) = \Delta s^r(\mathbf{x}_r) - Q^r(\mathbf{x}_r)$
- $s^{X_{-r}|X_r}(\mathbf{x}(t)) = -\ln(p_{\mathbf{x}(t)}(t)) + \ln(p_{\mathbf{x}_r(t)}(t))$
- $Q^{-r}(\mathbf{x}) = \sum_{i \notin r} Q^i(\mathbf{x})$

$$\sigma(\mathbf{x}) = \sigma^r(\mathbf{x}) + \Delta s^{X_{-r}|X_r}(\mathbf{x}) - Q^{-r}(\mathbf{x})$$

- Take expectation value and differentiate:

$$\langle\dot{\sigma}(t)\rangle = \langle\dot{\sigma}^r(t)\rangle + \langle\dot{\sigma}_{-r}(t)\rangle + \frac{d^r}{dt}S^{X|X_r}(t)$$

$$\langle\dot{\sigma}(t)\rangle = \langle\dot{\sigma}^r(t)\rangle + \langle\dot{\sigma}_{-r}(t)\rangle + \frac{d^r}{dt}S^{X|X_r}(t)$$

- The ***local EP rate*** is $\langle\dot{\sigma}^r(t)\rangle$
  - This term is ***non-negative***, and ***concerns an entire community***
  - The term "σ_X" in (*Sagawa and Shiraishi*, PRE, 2015) can be negative, and does not concern an entire community
  - The term "$\dot{S}_i^X$" in (*Horowitz and Esposito*, PRX, 2014) is non-negative, but does not concern an entire community
  - The term "σ_Ω" in (*Sagawa and Shiraishi*, PRE, 2015) is non-negative, but concerns a subset of possible transitions of global system

$$\langle \dot{\sigma}(t) \rangle = \langle \dot{\sigma}^r(t) \rangle + \langle \dot{\sigma}_{-r}(t) \rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

- $$\langle \dot{\sigma}_{-r}(t) \rangle = \sum_{x,x'} K_x^{x'}(-r;t) p_{x'}(t) \ln \left[\frac{K_x^{x'}(-r;t) p_{x'}(t)}{K_{x'}^{x}(-r;t) p_x(t)} \right]$$

  is a *system-wide* EP rate
  - just evaluated according to a ***counterfactual rate matrix***, $K(-r; t) = \sum_{i \notin r} K(i; \mathrm{t})$

- So this term ***is non-negative***

$$\langle\dot{\sigma}(t)\rangle = \langle\dot{\sigma}^r(t)\rangle + \langle\dot{\sigma}_{-r}(t)\rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

- $$\frac{d^r}{dt} S^{X|X_r}(t) = -\sum_{x,x'} K_x^{x'}(r;t) p_{x'}(t) \ln p_{x|x_r}(t)$$

  is a derivative of conditional entropy, just according to a counterfactual rate matrix.

- By data-processing inequality, *if r is a community*, this term ***is non-negative***

$$\langle\dot\sigma(t)\rangle = \langle\dot\sigma^r(t)\rangle + \langle\dot\sigma_{-r}(t)\rangle + \frac{d^r}{dt}S^{X|X_r}(t)$$

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- By data-processing inequality, *if r is a community*, this term ***is non-negative***

- If:
  1) Two subsystems, where *r* is one of those subsystems
  2) *r* is a community, i.e., it evolves independently
  3) Full system is at an NESS

  this term equals "learning rate" of (*Barato, Hartich, Seifert*, NJP, 2014)

$$\langle \dot{\sigma}(t) \rangle = \langle \dot{\sigma}^r(t) \rangle + \langle \dot{\sigma}_{-r}(t) \rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

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- By data-processing inequality, *if r is a community*, this term ***is non-negative***

- If:
  1) Two subsystems, where *r* is one of those subsystems
  2) Don't require *r* to be a community – so lose guarantee of non-negative EP

  this term equals "information flow" of (*Horowitz, Esposito*, PRX, 2014). (See also (*Sagawa, Ueda*, NJP, 2013).)

$$\langle \dot{\sigma}(t) \rangle = \langle \dot{\sigma}^r(t) \rangle + \langle \dot{\sigma}_{-r}(t) \rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

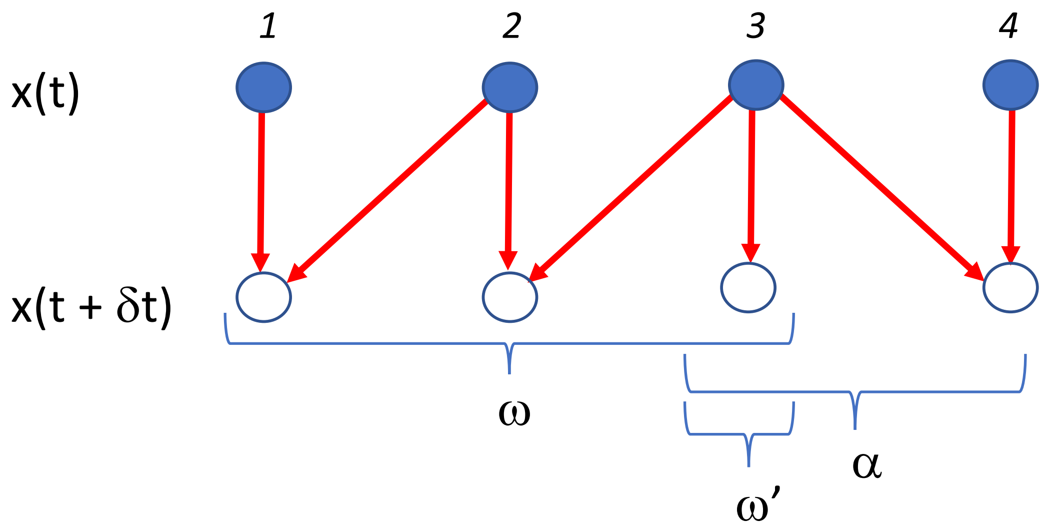
- $$\frac{d^r}{dt} S^{X|X_r}(t) = -\sum_{x,x'} K_x^{x'}(r;t) p_{x'}(t) \ln p_{x|x_r}(t)$$

  is a derivative of conditional entropy, just according to a counterfactual rate matrix.

- By data-processing inequality, this term ***is non-negative***

- If:
  1) Two subsystems, where *r* is one of those subsystems
  2) Both systems are communities, i.e., they evolve independently
  3) One system never changes state

  this term equals (time-derivative of) "Landauer loss" (*Wolpert, Kolchinsky*, NJP, 2020), aka "modularity dissipation" (*Boyd, Mandal, Crutchfield*, PRX, 2018)



- For any community r,

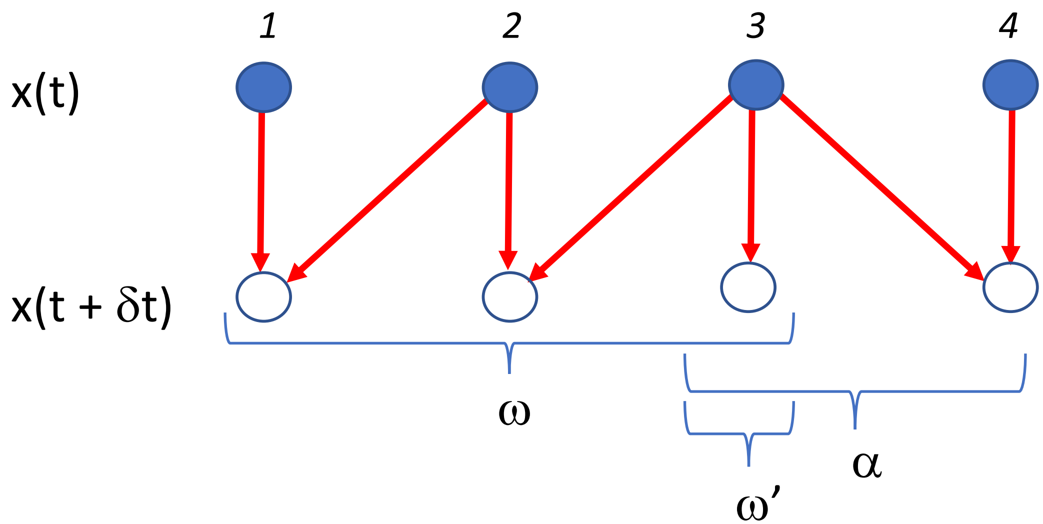
$$\langle \dot{\sigma}(t) \rangle = \langle \dot{\sigma}^r(t) \rangle + \langle \dot{\sigma}_{-r}(t) \rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

- All three terms on RHS are non-negative. So

$$\langle \dot{\sigma}(t) \rangle \geq \frac{d^r}{dt} S^{X|X_r}(t)$$

- Therefore in the example above,

$$\langle \dot{\sigma}(t) \rangle \geq \max \left[\frac{d^\omega}{dt} S^{X|X_\omega}(t), \frac{d^\alpha}{dt} S^{X|X_\alpha}(t), \frac{d^{\omega'}}{dt} S^{X|X_{\omega'}}(t) \right]$$



- For any community *r*,

$$\langle \dot{\sigma}(t) \rangle = \langle \dot{\sigma}^r(t) \rangle + \langle \dot{\sigma}_{-r}(t) \rangle + \frac{d^r}{dt} S^{X|X_r}(t)$$

- In the example above, ω' is a community within ω.

- So can "iterate" the full decomposition of expected EP rate, by decomposing $\langle \dot{\sigma}^\omega(t) \rangle$

- Therefore in the example above,

$$\langle \dot{\sigma}(t) \rangle \geq \frac{d^\omega}{dt} S^{X|X_\omega}(t) + \frac{d^{\omega'}}{dt} S^{X_\omega|X_{\omega'}}(t)$$

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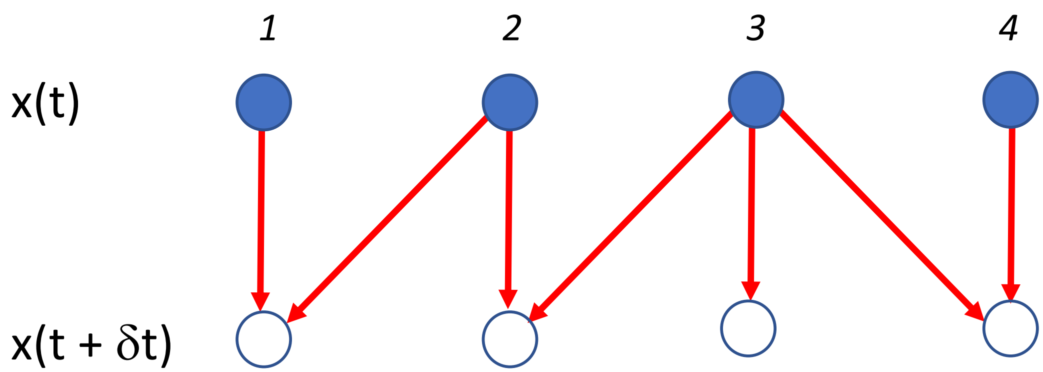

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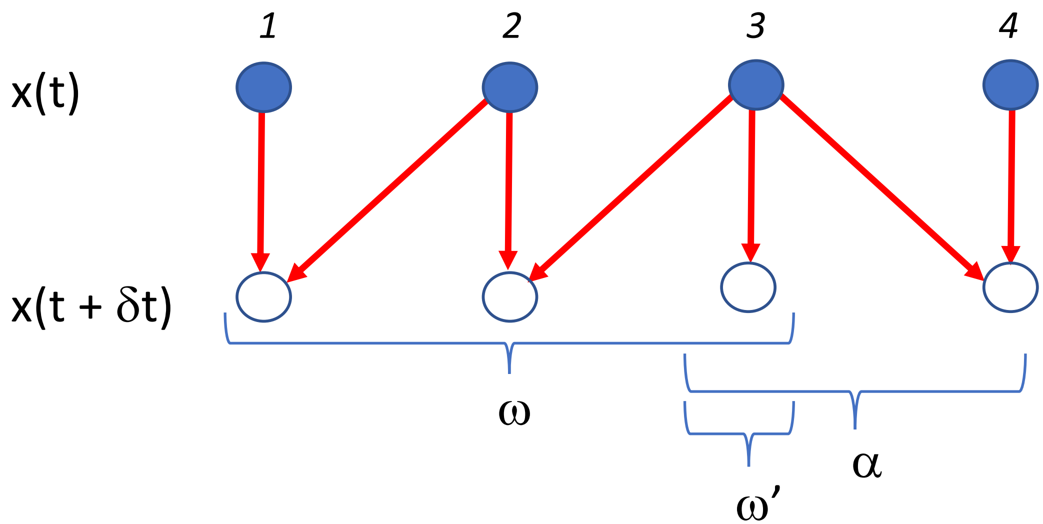


- ***System-wide heat flow*** during trajectory $\mathbf{x}$ is

$$Q(\mathbf{x}) = \sum_i Q^i(\mathbf{x}) = \widehat{\sum_r} Q^r(\mathbf{x}_r)$$

where ***inclusion-exclusion sum*** ("in-ex sum") is

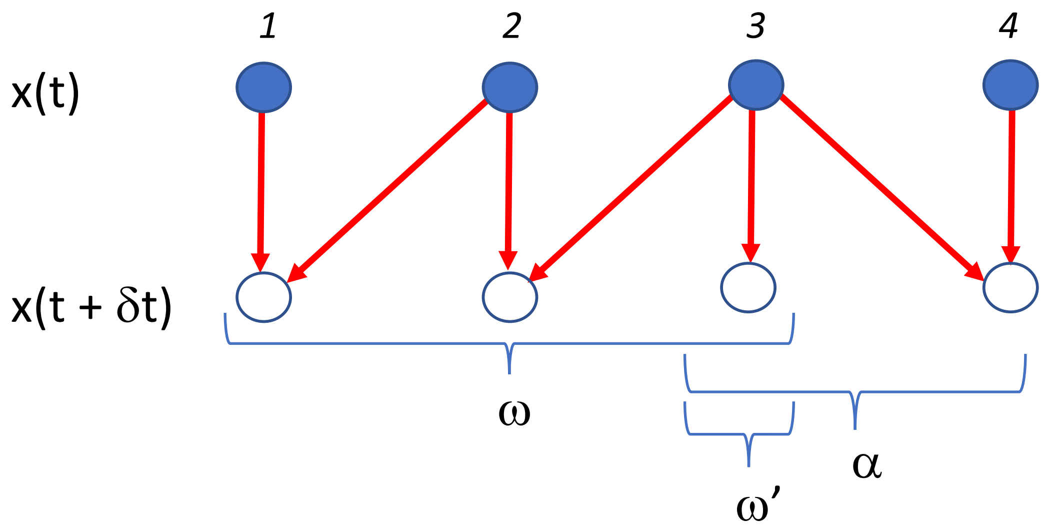
$$\widehat{\sum_r} Q^r(\mathbf{x}_r) = \sum_r Q^r(\mathbf{x}_r) - \sum_{r<r'} Q^{r\cap r'}(\mathbf{x}_r) + \ldots$$

- Therefore ***system-wide EP*** during trajectory $\mathbf{x}$ is

$$\sigma(\mathbf{x}) \;=\; \Delta s(\mathbf{x}) - Q(\mathbf{x}) \;=\; \widehat{\sum_r} \sigma^r(\mathbf{x}) - \Delta I^*(\mathbf{x})$$

where ***in-ex information*** is

$$I^*(\mathbf{x}(t)) = -s(\mathbf{x}(t)) + \widehat{\sum_r} s^r(\mathbf{x}(t))$$



- Conditional IFT:

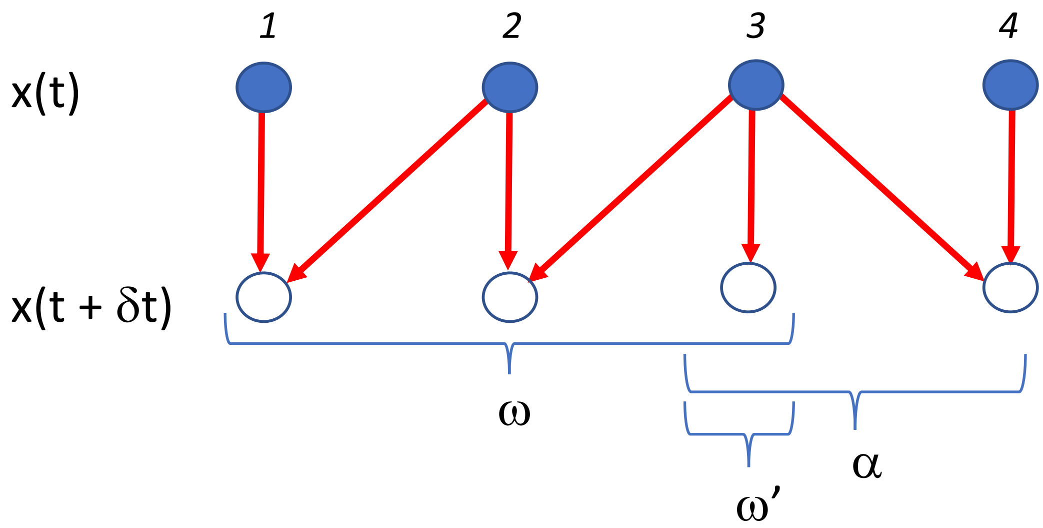
$$\langle e^{\sigma^r - \sigma} | \sigma^r \rangle = 1$$

- Second expansion of system-wide EP:

$$\sigma(\mathbf{x}) = \widehat{\sum_{r'}} \sigma^{r'}(\mathbf{x}) - \Delta I^*(\mathbf{x})$$

- Combining and applying Jensen's inequality shows that for any community r,

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



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

Example (taking r = subsystems 3 and 4):

$$\langle \sigma^{123} - \sigma^{3} + \sigma^{34} - \Delta s^{1234} - \Delta s^{123} + \Delta s^{3} - \Delta s^{34} \,|\, \sigma^{34} \rangle \geq \sigma^{34}$$

CONCLUSIONS

- Restrictions on dependencies of each subsystem's rate matrix
- ***Two system-wide decompositions of (trajectory-level) EP*** in terms of those restrictions
- ***Nonzero lower bounds on expected system-wide EP rate*** in terms of those restrictions
  - Extends results on "*learning rate*", "*Landauer loss*", (and versions of "*second law for feedback control*", "*second law for information processing*", etc.)
- ***Conditional fluctuation theorems***
  - If can observe EP of one subsystem, what is vector of EPs of other subsystems?
- Other lower bounds on expected EP rate, other conditional IFTs, etc.

arXiv:2003.11144, arXiv:2001.02205