

A *variational* approach to nonequilibrium thermodynamics

Kyoto Workshop on Quantum Thermodynamics and Stochastic Thermodynamics 2025

Roadmap

1. Introduction to the variational approach
2. Application: Thermodynamic inference
3. Application: Thermodynamic decompositions
4. Summary

Introduction



Nonequilibrium systems violate time-reversal symmetry

$$p(\text{Trajectory}) \neq \tilde{p}(\text{Trajectory})$$



Entropy production (EP)

Quantifies violation of time-reversal symmetry

Relative entropy between forward and reverse processes

EP as relative entropy: Stochastic processes

$p(\vec{x})$: probability of trajectory \vec{x}
under forward process

$\tilde{p}(\vec{x})$: probability of trajectory \vec{x}
under reverse process

Entropy production

$$\begin{aligned}\Sigma &= D(p||\tilde{p}) \\ &= \left\langle \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})} \right\rangle_p \equiv \langle \sigma(\vec{x}) \rangle_p\end{aligned}$$

Donsker-Varadhan Variational Representation

$$\Sigma = D(p||\tilde{p}) = \sup_{g:\vec{x}\rightarrow\mathbb{R}} \langle g \rangle_p - \ln \langle e^g \rangle_{\tilde{p}}$$

Optimal: $g^*(\vec{x}) = \sigma(\vec{x}) := \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})}$

Interpretation as thermodynamic uncertainty relation (TUR)

$$\Sigma \geq \underbrace{(\langle g \rangle_p - \langle g \rangle_{\tilde{p}})}_{\text{Mean difference}} - \underbrace{\ln \langle e^{g - \langle g \rangle_{\tilde{p}}} \rangle_{\tilde{p}}}_{\text{Fluctuations}}$$

EPR as relative entropy: discrete short-time dynamics

Fluxes (one-way)

$$\mathbf{j} = (j_1, \dots, j_m) \in \mathbb{R}_+^m$$

Reverse fluxes

$$\tilde{\mathbf{j}} = (j_{-1}, \dots, j_{-m}) \in \mathbb{R}_+^m$$

Thermodynamic forces (forces)

$$\mathbf{f} := \left(\ln \frac{j_1}{j_{-1}}, \dots, \ln \frac{j_m}{j_{-m}} \right)$$

Entropy production rate

$$\begin{aligned} \dot{\Sigma} &= D(\mathbf{j} \parallel \tilde{\mathbf{j}}) \\ &= \sum_{\rho} j_{\rho} \ln \frac{j_{\rho}}{\tilde{j}_{\rho}} - j_{\rho} + \tilde{j}_{\rho} \end{aligned}$$

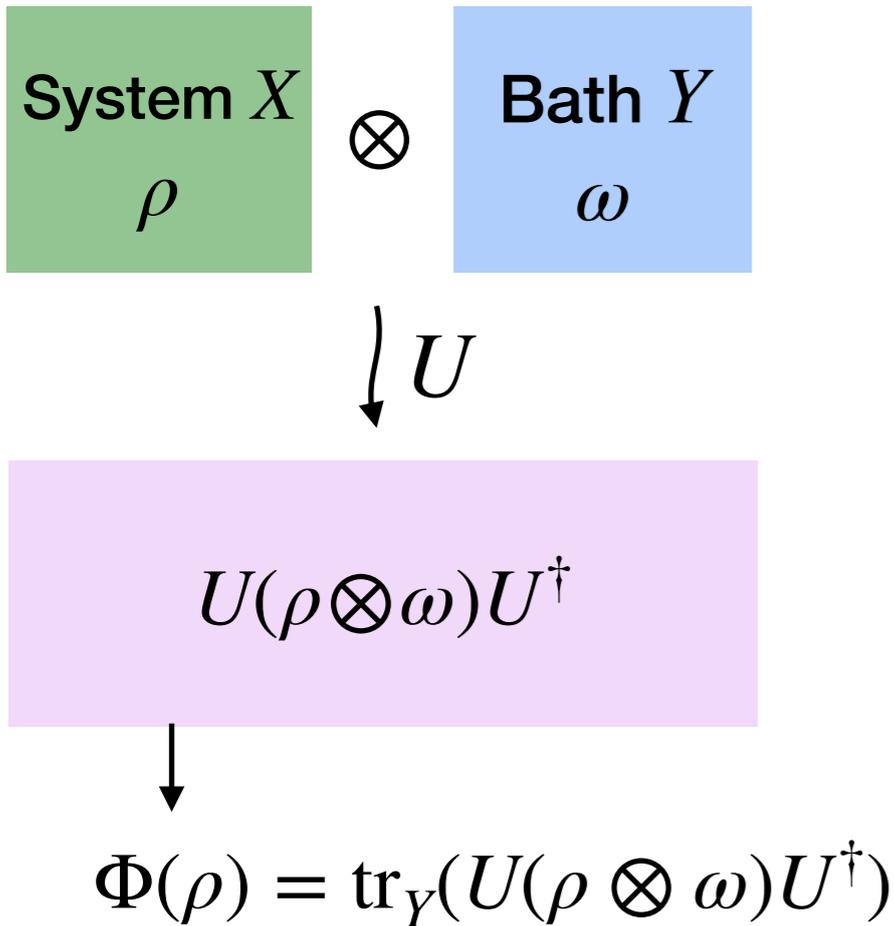
Donsker-Varadhan Variational Representation

$$\dot{\Sigma} = \max_{\boldsymbol{\theta} \in \mathbb{R}^m} \mathbf{j}^{\top} \boldsymbol{\theta} - \tilde{\mathbf{j}}^{\top} (e^{\boldsymbol{\theta}} - 1)$$

Optimal: $\theta_{\rho}^* = f_{\rho} := \ln \frac{j_{\rho}}{\tilde{j}_{\rho}}$

EP as relative entropy: quantum systems

Inclusive Hamiltonian approach



Entropy production

$$\Sigma = S[U(\rho \otimes \omega)U^\dagger \parallel \Phi(\rho) \otimes \omega]$$

Esposito, Lindenberg, Van den Broeck, *NJP*, 2010

Flux-force form

$$\Sigma = \text{tr}\{U(\rho \otimes \omega)U^\dagger F\}$$

Force operator

$$F := \ln U(\rho \otimes \omega)U^\dagger - \ln \Phi(\rho) \otimes \omega$$

Variational Representation

$$\Sigma = \max_{A \in \mathcal{H}_{XY}} [\text{tr}\{U(\rho \otimes \omega)U^\dagger A\} - \ln \text{tr}\{e^{\ln(\Phi(\rho) \otimes \omega) + A}\}]$$

$$A^* = F$$

Summary

Stochastic Processes

$$\Sigma = \sup_g \langle g \rangle_p - \ln \langle e^g \rangle_{\tilde{p}}$$

Discrete dynamics

$$\dot{\Sigma} = \max_{\theta} \mathbf{j}^T \boldsymbol{\theta} - \tilde{\mathbf{j}}^T (e^{\boldsymbol{\theta}} - 1)$$

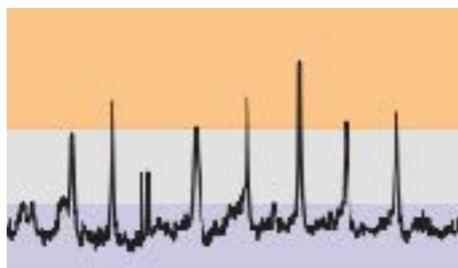
Quantum

$$\Sigma = \max_A \left[\text{tr} \{ U(\rho \otimes \omega) U^\dagger A \} - \ln \text{tr} \{ e^{\ln(\Phi(\rho) \otimes \omega) + A} \} \right]$$

Applications

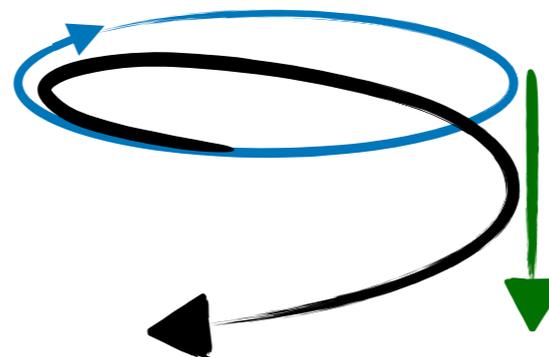
Thermodynamic
inference

$$\hat{\Sigma} = f(\text{measurements})$$



Thermodynamic
Decompositions

$$\Sigma = \Sigma_1 + \Sigma_2$$



TURs & thermodynamic
speed limits

$$\Sigma \geq f(\text{Speed})$$



Application 1: Thermodynamic inference

Inferring entropy production in many-body systems using nonequilibrium MaxEnt

Miguel Aguilera,^{1,2,*} Sosuke Ito,^{3,4} and Artemy Kolchinsky^{5,3,†}

[arXiv:2505.10444](https://arxiv.org/abs/2505.10444)



Miguel Aguilera

Basque Center of Applied Mathematics

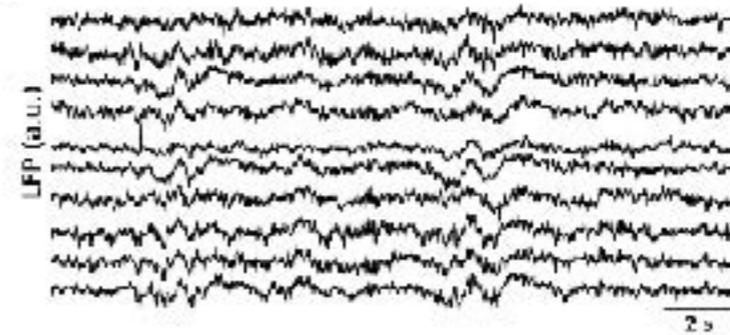


Sosuke Ito

University of Tokyo

Thermodynamic inference

Time series
data



Average EP $\Sigma := D(p(\vec{x}) || \tilde{p}(\vec{x})) = \langle \sigma \rangle_p$

Fluctuating EP $\sigma(\vec{x}) := \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})}$

High-dimensional systems

long non-Markovian memory and/or many degrees of freedom

Average EP

$$\Sigma := D[p(\vec{x}) || \tilde{p}(\vec{x})] = \langle \sigma \rangle_p$$

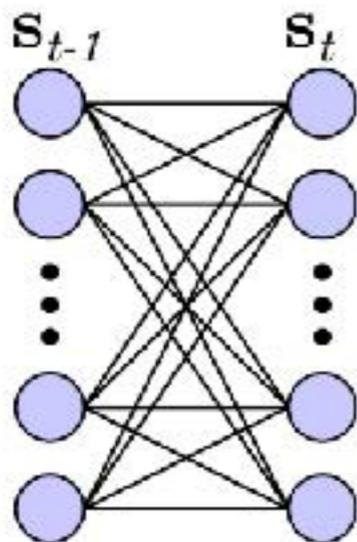
Fluctuating EP

$$\sigma(\vec{x}) := \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})}$$

Trajectory over $T \gg 1$ steps: $\vec{x} = (x_0, x_1, \dots, x_T)$

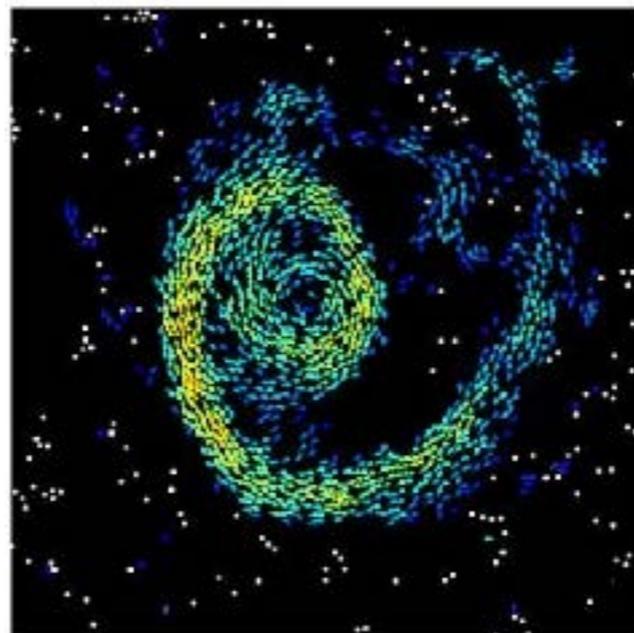
$N \gg 1$ degrees of freedom: $x_t = (x_{0,t}, x_{1,t}, \dots, x_{N,t})$

Nonequilibrium spin glass



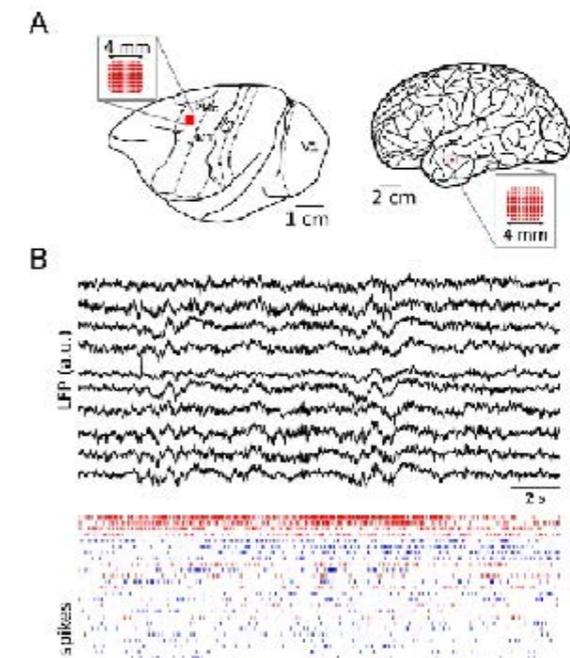
10.1038/s41467-023-39107-y

Active matter



10.1073/pnas.2104724118

Biological and neural systems



10.1038/srep40211

High-dimensional systems

nonstationary, long non-Markovian memory, and/or many degrees of freedom

Average EP

$$\Sigma := D[p(\vec{x}) || \tilde{p}(\vec{x})] = \langle \sigma \rangle_p$$

Fluctuating EP

$$\sigma(\vec{x}) := \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})}$$

Trajectory over $T \gg 1$ steps: $\vec{x} = (x_0, x_1, \dots, x_T)$

$N \gg 1$ degrees of freedom: $x_t = (x_{0,t}, x_{1,t}, \dots, x_{N,t})$

Challenges for thermodynamic inference

Statistically impossible to infer trajectory distributions p and \tilde{p}
(e.g., $\sim 2^{(T+1)N}$ parameters for a system with N binary spins)

Computationally intractable to evaluate KL divergence

EP bound from statistics of observable

Trajectories characterized
by vector of d observables

$$\vec{x} \mapsto \mathbf{g}(\vec{x}) \in \mathbb{R}^d$$

Example: $N(N - 1)/2$ antisymmetric
cross-correlations over 1 time-step:

$$g_{ij}(\vec{x}) = x_{i,1}x_{j,0} - x_{j,1}x_{i,0}$$

Dissipation due to observables \mathbf{g}

$$\Sigma_{\mathbf{g}} := \min_q D[q(\vec{x}) \parallel \tilde{p}(\vec{x})] \quad \text{such that} \quad \langle \mathbf{g} \rangle_q = \langle \mathbf{g} \rangle_p$$

- Lower bound: $\Sigma_{\mathbf{g}} \leq \Sigma = D[p(\vec{x}) \parallel \tilde{p}(\vec{x})]$
- Space of trajectory distributions q is exponentially large
→ Intractable constrained optimization problem
- “Prior” distribution $\tilde{p}(\vec{x})$ not known in closed form

Convex duality

$$\Sigma_g = \min_q D[q(\vec{x}) || \tilde{p}(\vec{x})]$$

such that $\langle \mathbf{g} \rangle_q = \langle \mathbf{g} \rangle_p$

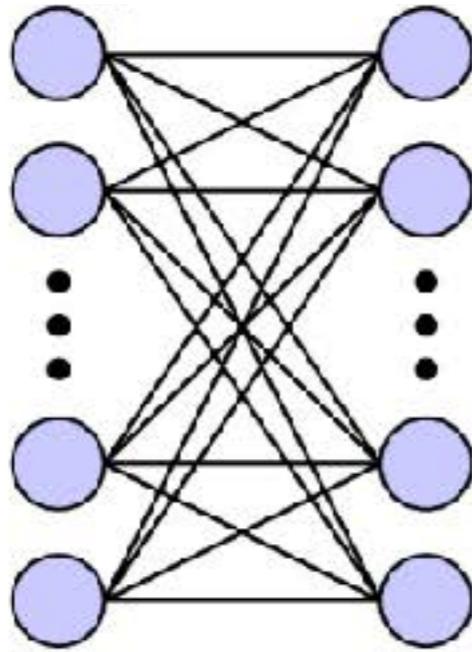
Dual problem

$$\Sigma_g = \max_{\theta \in \mathbb{R}^d} \theta^\top \langle \mathbf{g} \rangle_p - \ln \langle e^{\theta^\top \mathbf{g}} \rangle_{\tilde{p}}$$

Donsker-Varadhan representation!

- Low-dimensional unconstrained convex optimization problem
- No inference of trajectory probabilities, only expectations
- Obeys the bounds $0 \leq \Sigma_g \leq \Sigma$
- Estimate of fluctuating EP: $\sigma(\vec{x}) = \ln \frac{p(\vec{x})}{\tilde{p}(\vec{x})} \approx \theta^{*\top} \mathbf{g}(\vec{x})$

Example: Nonequilibrium kinetic Ising model



Multipartite dynamics

$$T(\mathbf{x}_1|\mathbf{x}_0) = \frac{1}{N} \sum_i \left[W_i(\mathbf{x}_0) \delta_{\mathbf{x}_0, \mathbf{x}_1^{[i]}} + (1 - W_i(\mathbf{x}_0)) \delta_{\mathbf{x}_0, \mathbf{x}_1} \right]$$

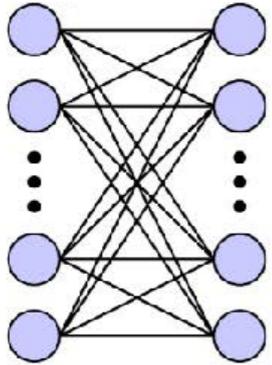
Spin-flip probability

$$W_i(\mathbf{x}) = \frac{\exp(-\beta x_i \sum_j w_{ij} x_j)}{2 \cosh(\beta \sum_j w_{ij} x_j)}$$

$$\Sigma = \frac{\beta}{2} \sum_{i>j} (w_{ij} - w_{ji}) \langle g_{ij}(\mathbf{x}) \rangle$$

$$g_{ij}(\mathbf{x}) = x_{i,1} x_{j,0} - x_{j,1} x_{i,0}$$

Example: Nonequilibrium kinetic Ising model



Spin-flip probability

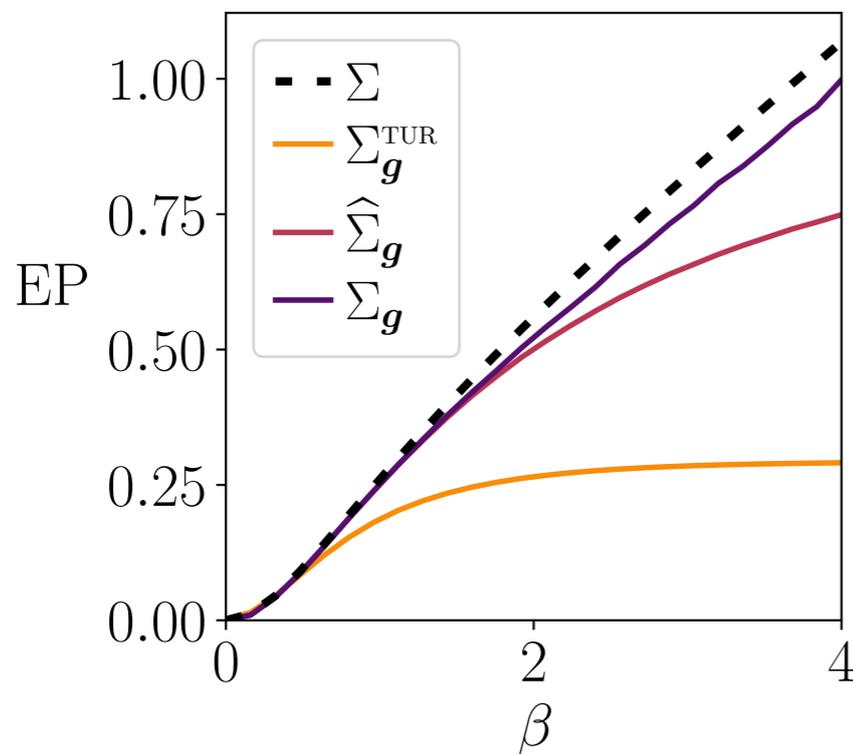
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$$\Sigma = \frac{\beta}{2} \sum_{i>j} (w_{ij} - w_{ji}) \langle g_{ij}(\mathbf{x}) \rangle$$

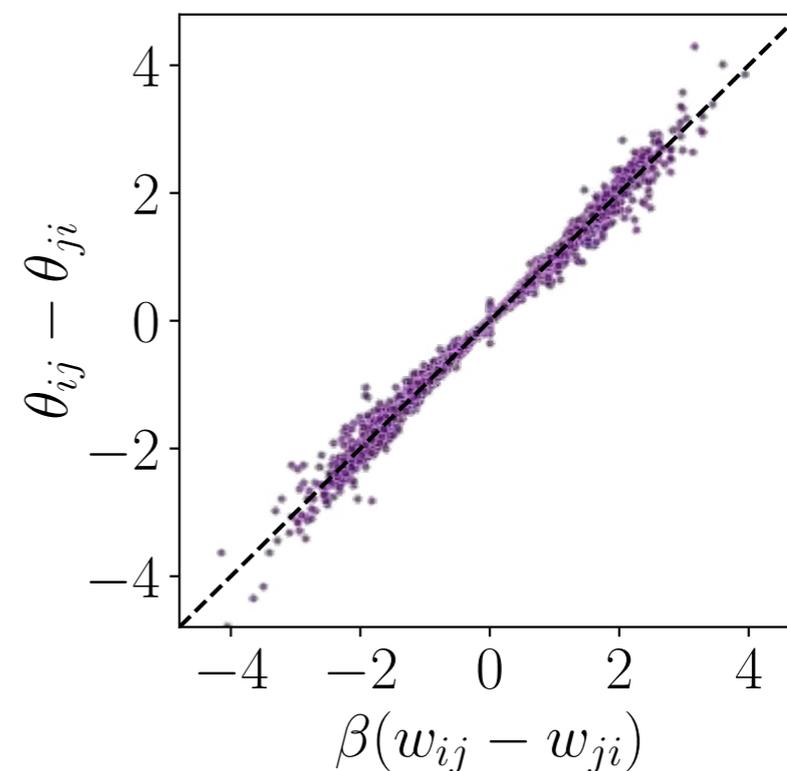
$$g_{ij}(\mathbf{x}) = x_{i,1} x_{j,0} - x_{j,1} x_{i,0}$$

Inference on $N = 1000$ spin system (10^9 samples)

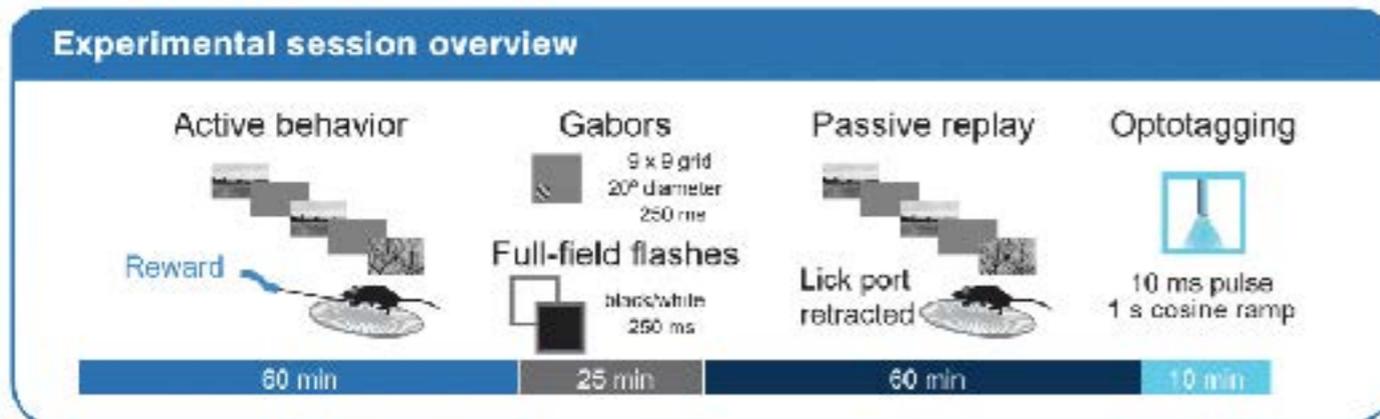
Average EP



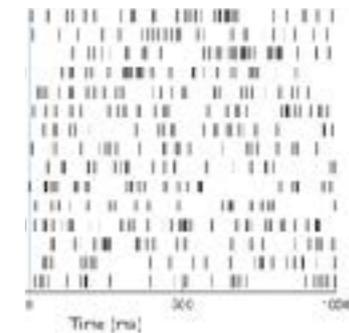
Parameter inference



Example: Real-world neural data

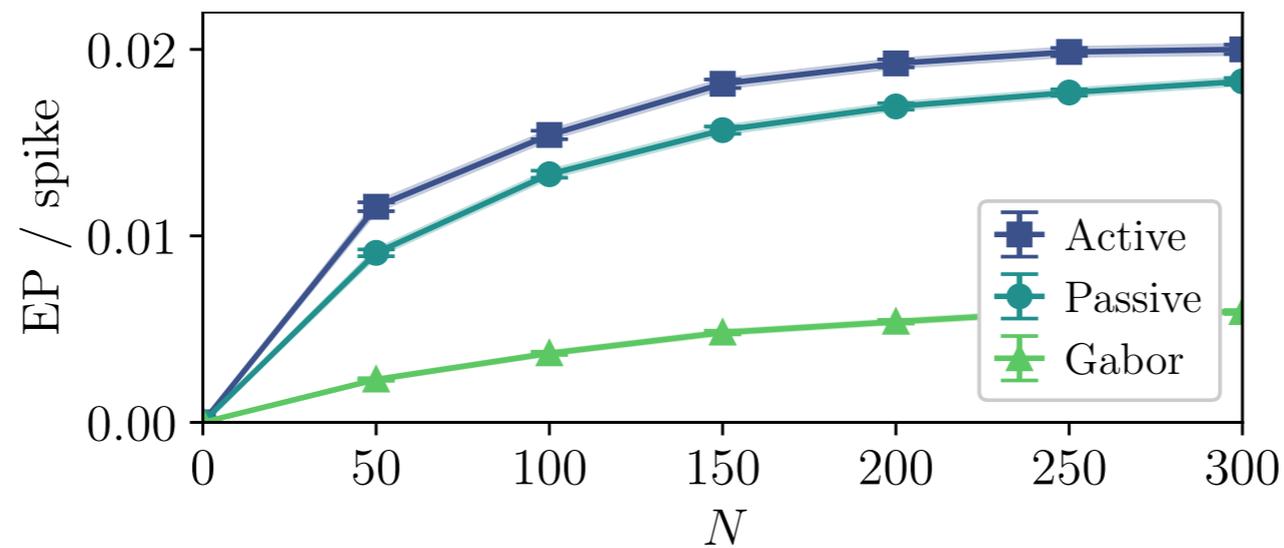


Spike data (500 neurons)



$$g_{ij}(\vec{x}) = x_{i,1} x_{j,0} - x_{i,0} x_{j,1}$$

Average EP / spike



Summary

Inferring entropy production in many-body systems using nonequilibrium MaxEnt

Miguel Aguilera,^{1,2,*} Sosuke Ito,^{3,4} and Artemy Kolchinsky^{5,3,†}

- Variational method allows inference EP in high-dimensional systems
- Future work: hierarchical decomposition

k-point correlations

$$g^{(k)}(\vec{x}) = \left\{ \prod_{(i,t) \in S} x_{i,t} : S \subseteq V : |S| = k \right\}$$

Hierarchical decomposition of EP

$$0 \leq \Sigma_{(1)} \leq \Sigma_{(2)} \leq \Sigma_{(3)} \leq \dots \leq \Sigma$$

Thermodynamic Inference: open problem

Formal Limitations on the Measurement of Mutual Information

David McAllester
Toyota Technological Institute at Chicago

Karl Stratos
Rutgers University

Proc of Machine Learning Research, 2020

Takeaway: distribution-free lower bounds on relative entropy cannot be accurate when $D_{KL} \gg \ln N$, where N is number of samples.

- Does this limitation apply to variational inference of EP?
- Can any distribution-free method infer EP values of $\Sigma \gg \ln N$?
- Are there “no-go theorems” for thermodynamic inference?

Application 2: Thermodynamic decompositions

EPR as relative entropy: discrete short-time dynamics

Fluxes (one-way)

$$\mathbf{j} = (j_1, \dots, j_m) \in \mathbb{R}_+^m$$

Reverse fluxes

$$\tilde{\mathbf{j}} = (j_{-1}, \dots, j_{-m}) \in \mathbb{R}_+^m$$

Thermodynamic forces (forces)

$$\mathbf{f} := \left(\ln \frac{j_1}{j_{-1}}, \dots, \ln \frac{j_m}{j_{-m}} \right)$$

Entropy production rate

$$\begin{aligned} \dot{\Sigma} &= D(\mathbf{j} \parallel \tilde{\mathbf{j}}) \\ &= \sum_{\rho} j_{\rho} \ln \frac{j_{\rho}}{\tilde{j}_{\rho}} - j_{\rho} + \tilde{j}_{\rho} \end{aligned}$$

Variational Representation

$$\dot{\Sigma} = \max_{\boldsymbol{\theta} \in \mathbb{R}^m} \mathbf{j}^{\top} \boldsymbol{\theta} - \tilde{\mathbf{j}}^{\top} (e^{\boldsymbol{\theta}} - 1)$$

$$\text{Optimal: } \theta_{\rho}^* = f_{\rho} := \ln \frac{j_{\rho}}{\tilde{j}_{\rho}}$$

Optimization restricted to subset $\Theta \subseteq \mathbb{R}^m$

$$\dot{\Sigma} = \max_{\theta \in \mathbb{R}^m} j^\top \theta - \tilde{j}^\top (e^\theta - 1)$$

$$\dot{\Sigma}_\Theta = \max_{\theta \in \Theta} j^\top \theta - \tilde{j}^\top (e^\theta - 1)$$

Decomposition of EP

$$\dot{\Sigma} = \dot{\Sigma}_\Theta + \cancel{\dot{\Sigma}_{\perp\Theta}}$$

$\dot{\Sigma}_\Theta$: contribution from forces inside Θ

$\dot{\Sigma}_{\perp\Theta}$: contribution from forces outside Θ

Decomposition of forces

$$f = \underbrace{\theta^*}_{\text{Inside } \Theta} + \underbrace{\cancel{f - \theta^*}}_{\text{Outside } \Theta}$$

θ^* is “best approximation” of f

Decomposition of fluxes

$$j = \underbrace{\tilde{j} \circ e^{\theta^*}}_{\text{Inside } \Theta} + \underbrace{\cancel{j - \tilde{j} \circ e^{\theta^*}}}_{\text{Outside } \Theta}$$

When $f \in \Theta$,
“outside” terms vanish

Special case: Θ is a d -dimensional linear subspace

$$\Theta = \{M\phi : \phi \in \mathbb{R}^d\}$$

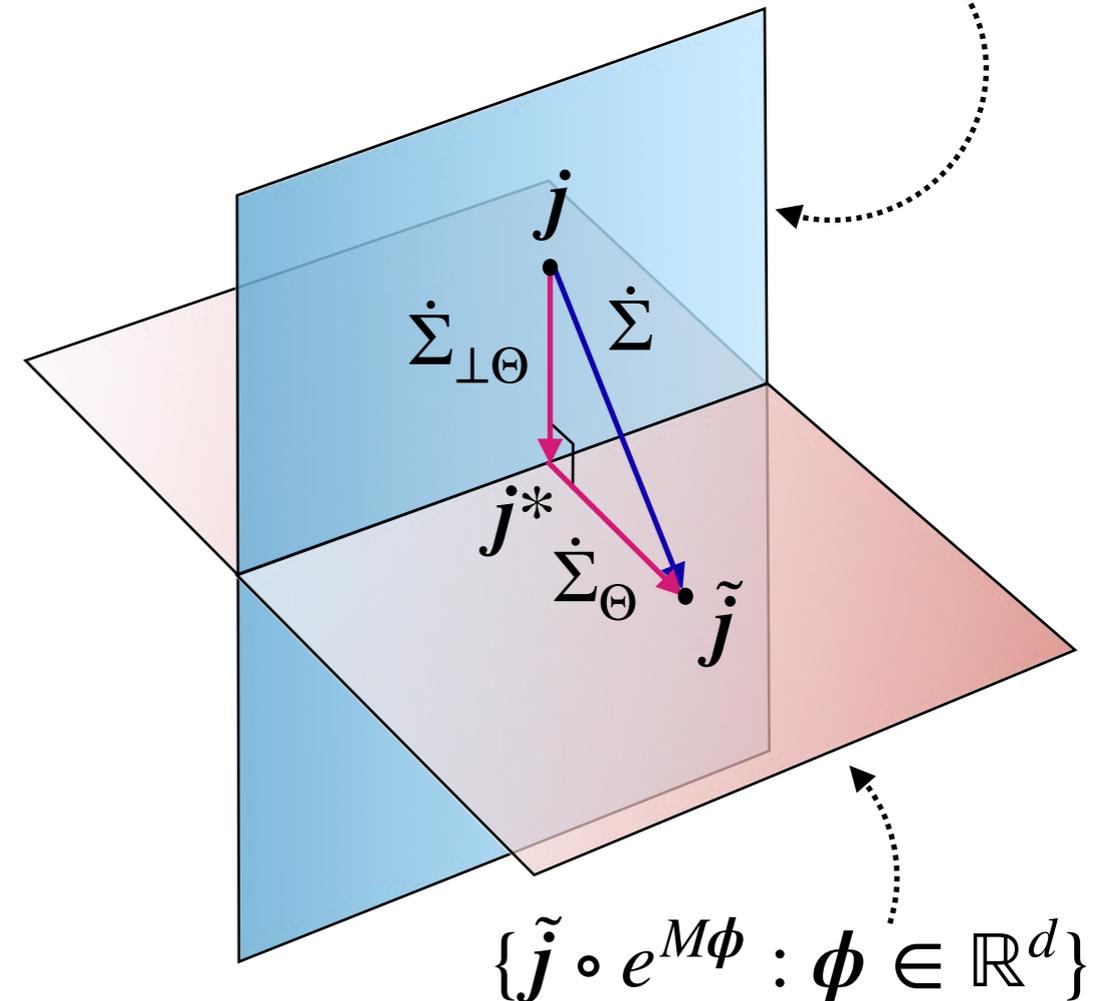
$$\{j' : M^\top j' = M^\top j\}$$

Convex Duality

$$\dot{\Sigma}_\Theta = \max_{\phi \in \mathbb{R}^d} j^\top M\phi - \tilde{j}^\top (e^{M\phi} - 1)$$

$$= \min_{j' \in \mathbb{R}_+^m} D(j' \| \tilde{j}) \text{ where } M^\top j' = M^\top j$$

$$j^* = \tilde{j} \circ e^{M\phi^*}$$



Decomposition of fluxes

$$j = \underbrace{j^*}_{\text{Within subspace}} + \underbrace{(j - j^*)}_{\text{Outside subspace}}$$

Within subspace Outside subspace

Pythagorean Decomposition of EP

$$D(j \| \tilde{j}) = D(j^* \| \tilde{j}) + D(j \| j^*)$$

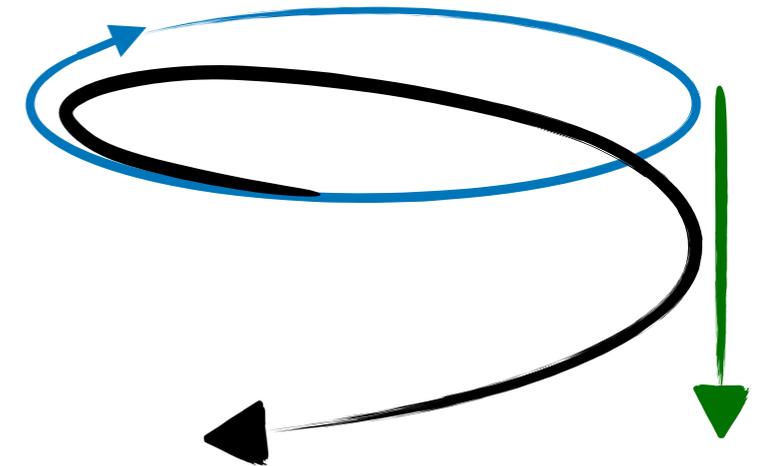
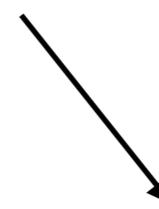
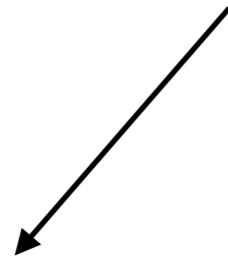
$$\underbrace{\hspace{10em}}_{\dot{\Sigma}}$$

$$\underbrace{\hspace{10em}}_{\dot{\Sigma}_\Theta}$$

$$\underbrace{\hspace{10em}}_{\dot{\Sigma}_{\perp\Theta}}$$

Case study: Excess vs. housekeeping decomposition

$$\dot{\Sigma} = \dot{\Sigma}_{hk} + \dot{\Sigma}_{ex}$$



Housekeeping

Nonconservative contribution
Associated w/ stationary cyclic fluxes

Excess

Conservative contribution
Associated w/ free energy potential
Non-stationary contribution

Is it possible to define a general and operationally meaningful decomposition?

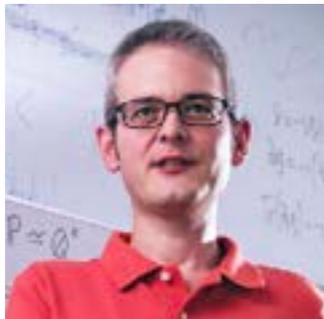
Case study: Excess vs. housekeeping decomposition

Generalized free energy and excess entropy production for active systems

Artemy Kolchinsky,^{1,2} Andreas Dechant,³ Kohei Yoshimura,⁴ and Sosuke Ito^{2,4}

[arXiv:2412.08432](https://arxiv.org/abs/2412.08432)

Andreas Dechant



Kohei Yoshimura



Sosuke Ito



Case study: Excess vs. housekeeping decomposition

Dynamics

$$\dot{\mathbf{x}}(t) = \nabla^\top \mathbf{j} - \mathbf{v}^{\text{ext}}$$

(discrete continuity equation)

$\mathbf{x} \in \mathbb{R}_+^n$: distribution/concentration vector

$\mathbf{j} \in \mathbb{R}_+^m$: forward one-way fluxes

$\nabla \in \mathbb{Z}^{m \times n}$: stoichiometric matrix

\mathbf{v}^{ext} : external fluxes

Passive systems

relax to equilibrium
conservative forces

$$f := \ln \frac{\dot{\mathbf{j}}}{\tilde{\mathbf{j}}} = -\nabla \phi^{\text{eq}}$$

$$\phi_i^{\text{eq}} = \ln \frac{x_i}{x_i^{\text{eq}}} = \partial_{x_i} D(\mathbf{x} || \mathbf{x}^{\text{eq}})$$

Active systems

relax to NESS / limit cycles / chaos
nonconservative forces

$$f := \ln \frac{\dot{\mathbf{j}}}{\tilde{\mathbf{j}}} \neq -\nabla \phi \quad \text{for any } \phi$$

Case study: Excess vs. housekeeping decomposition

$$\dot{\Sigma} = \max_{\theta \in \mathbb{R}^m} \mathbf{j}^\top \boldsymbol{\theta} - \tilde{\mathbf{j}}^\top (e^\theta - 1)$$

conservative forces

$$\mathbf{f} = -\nabla \phi^{\text{eq}}$$

Restricted optimization

over span of matrix $-\nabla$

$$\dot{\Sigma}_{\text{ex}} = \max_{\phi \in \mathbb{R}^n} -\mathbf{j}^\top \nabla \phi - \tilde{\mathbf{j}}^\top (e^{-\nabla \phi} - 1)$$

ϕ^* is generalized free energy

Case study: Excess vs. housekeeping decomposition

$$\dot{\Sigma}_{\text{ex}} = \max_{\phi \in \mathbb{R}^n} -\mathbf{j}^\top \nabla \phi - \tilde{\mathbf{j}}^\top (e^{-\nabla \phi} - 1)$$

$$\mathbf{j}^* = \tilde{\mathbf{j}} \circ e^{-\nabla \phi^*}$$

For system without external fluxes, excess EPR vanishes in stationarity

$$\dot{\Sigma}_{\text{ex}} = \min_{\mathbf{j}' \in \mathbb{R}_+^m} D(\mathbf{j}' \| \tilde{\mathbf{j}}) \quad \text{where} \quad \nabla^\top \mathbf{j}' = \nabla^\top \tilde{\mathbf{j}}$$

Decomposition of EP

$$\dot{\Sigma} = \dot{\Sigma}_{\text{ex}} + \dot{\Sigma}_{\text{hk}}$$

Decomposition of fluxes

$$\mathbf{j} = \underbrace{\mathbf{j}^*}_{\text{Nonstationary flux}} + \underbrace{(\mathbf{j} - \mathbf{j}^*)}_{\text{Cyclic flux}}$$

Decomposition of forces

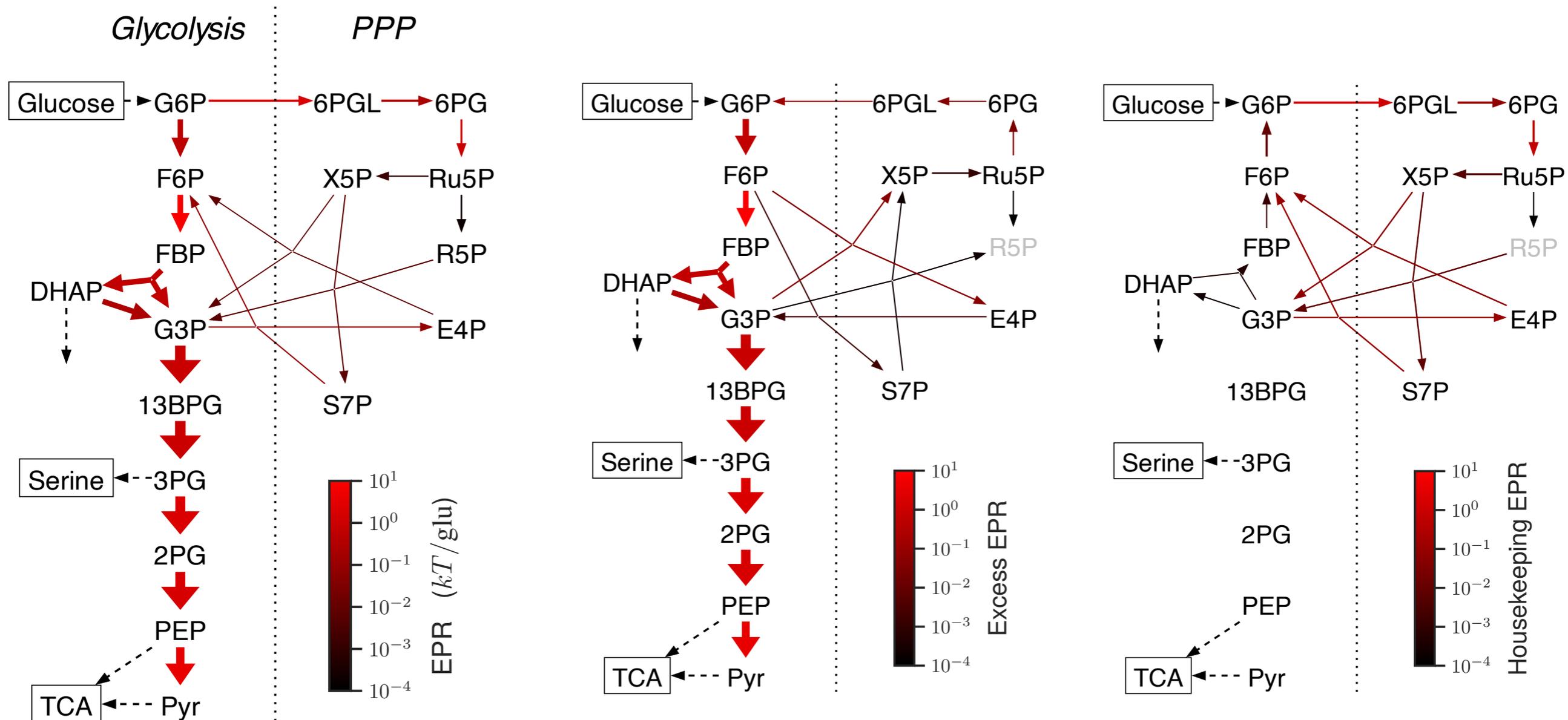
$$\mathbf{f} = \underbrace{-\nabla \phi^*}_{\text{Conservative}} + \underbrace{(\mathbf{f} + \nabla \phi^*)}_{\text{Nonconservative}}$$

Excess vs. housekeeping: Metabolic network example

E. Coli metabolism net fluxes

excess fluxes

housekeeping fluxes



Thermodynamic speed limit for steady-state open systems

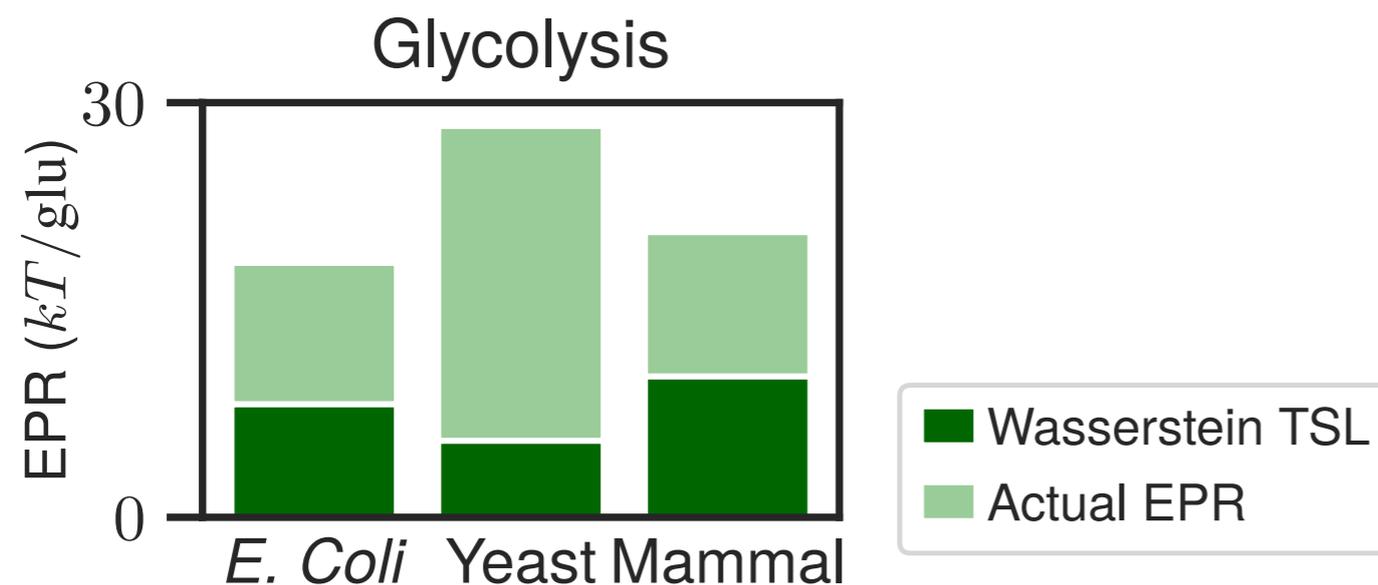
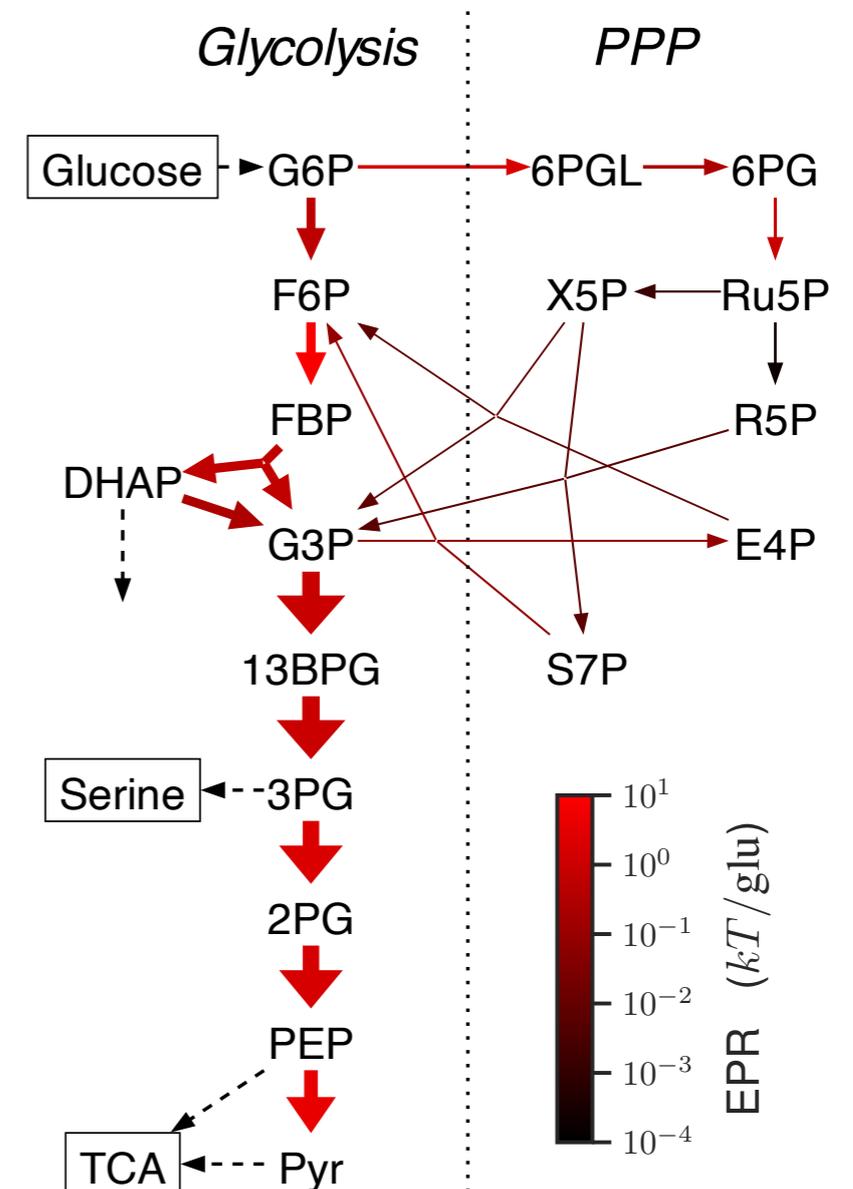
Optimal EPR

$$\dot{\Sigma}_{\text{TSL}} = \min_{j' \in \mathbb{R}_+^m} \dot{\Sigma}_{\text{ex}}(j') \quad \text{where} \quad \nabla^\top j' = \nu^{\text{ext}}, \quad \sum j'_\rho = A$$

Minimal excess EPR given fixed external fluxes ν^{ext}
and dynamical activity $A = \sum j_\rho$

$\dot{\Sigma}_{\text{TSL}}$ closely related to 1-Wasserstein distance

E. Coli metabolism



Preview: excess/housekeeping for quantum systems

(in preparation)

Ryusuke Hamazaki



Kohei Yoshimura



Sosuke Ito



Entropy production

$$\begin{aligned}\Sigma(\rho) &= S[U(\rho \otimes \omega)U^\dagger \| \Phi(\rho) \otimes \omega] \\ &= \text{tr}\{U(\rho \otimes \omega)U^\dagger F\}\end{aligned}$$

Force operator

$$F := \ln U(\rho \otimes \omega)U^\dagger - \ln \Phi(\rho) \otimes \omega$$

Variational Representation

$$\Sigma(\rho) = \max_{A \in \mathcal{H}_{XY}} [\text{tr}\{U(\rho \otimes \omega)U^\dagger A\} - \ln \text{tr}\{e^{\ln(\Phi(\rho) \otimes \omega) + A}\}]$$

Preview: excess/housekeeping for quantum systems

Entropy production

$$\begin{aligned}\Sigma(\rho) &= S[U(\rho \otimes \omega)U^\dagger \parallel \Phi(\rho) \otimes \omega] \\ &= \text{tr}\{U(\rho \otimes \omega)U^\dagger F\}\end{aligned}$$

$$F := \ln U(\rho \otimes \omega)U^\dagger - \ln \Phi(\rho) \otimes \omega$$

Variational Representation

$$\Sigma(\rho) = \max_{A \in \mathcal{H}_{XY}} \left[\text{tr}\{U(\rho \otimes \omega)U^\dagger A\} - \ln \text{tr}\{e^{\ln(\Phi(\rho) \otimes \omega) + A}\} \right]$$

Definition: conservative system

if $\Sigma(\rho) = 0$ for some ρ

Result: System is conservative iff force belongs to linear subspace

$$F \in \Omega_{\text{cons}} := \{U(L \otimes \mathbb{1}_Y)U^\dagger - M \otimes \mathbb{1}_Y, L \in \mathcal{H}_X, M \in \mathcal{H}_X\}$$

Definition of excess EP

$$\Sigma_{\text{ex}}(\rho) := \max_{A \in \Omega_{\text{cons}}} \left[\text{tr}\{U(\rho \otimes \omega)U^\dagger A\} - \ln \text{tr}\{e^{\ln(\Phi(\rho) \otimes \omega) + A}\} \right]$$

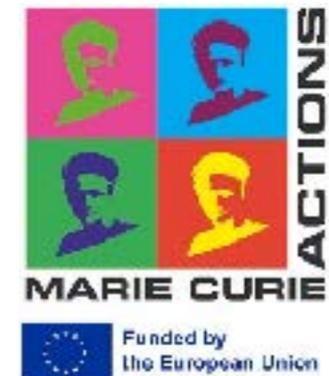
(in preparation)

Summary and thanks

- Variational expression of EP useful for thermodynamic inference, thermodynamic decompositions, and thermodynamic bounds (TUR/TSL)
- Unified formalism for continuous/discrete, Markovian/non-Markovian, classical/quantum systems

Collaborators

Miguel Aguilera
Andreas Dechant
Ryusuke Hamazaki
Sosuke Ito
Kohei Yoshimura



Supplemental Material

Open problem: uniqueness result

$$\dot{\Sigma}_{\text{ex}} = \max_{\phi \in \mathbb{R}^n} -\mathbf{j}^\top \nabla \phi - \tilde{\mathbf{j}}^\top (e^{-\nabla \phi} - 1)$$

Alternative variational excess EPR definitions have been proposed...

Housekeeping and excess entropy production for general nonlinear dynamics

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$$\dot{\Sigma}_{\text{ex}}^{\text{ons}} = \max_{\phi \in \mathbb{R}^n} -2\mathbf{j}^\top \nabla \phi - \phi^\top \nabla^\top L \nabla \phi \quad L_{\rho\rho} = \frac{(j_\rho - \tilde{j}_\rho)/2}{\ln j_\rho - \ln \tilde{j}_\rho}$$

Hessian geometry of nonequilibrium chemical reaction networks and entropy production decompositions

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Is there a “right” definition that uniquely satisfied desired properties?

Comparison to Kim-Otsubo variational principle

Donsker-Varadhan form

$$\Sigma_g = \max_{\theta \in \mathbb{R}^d} \theta^\top \langle \mathbf{g} \rangle_p - \ln \langle e^{\theta^\top \mathbf{g}} \rangle_{\tilde{p}}$$

Kim-Otsubo variational form

$$\Sigma_g^{\text{KO}} = \max_{\theta \in \mathbb{R}^d} \theta^\top \langle \mathbf{g} \rangle_p - \langle e^{\theta^\top \mathbf{g}} - 1 \rangle_{\tilde{p}}$$

Kim et al., Jeong, H. *PRL* 2020.
Otsubo, et al, *Comm Physics*, 2022.

Donsker-Varadhan
bound is always tighter:

$$\Sigma_g \geq \Sigma_g^{\text{KO}}$$

