Geometric thermodynamics: Nonequilibrium thermodynamics based on optimal transport and information geometry

Statphys 28, 8th Aug. 2023

Sosuke Ito* (Universal Biology Institute, UTokyo), Andreas Dechant (KyotoU), Shin-ichi Sasa (KyotoU), and Muka Nakazato (UTokyo)

*Speaker

This talk [T2-08A-04]

[Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).
[Dechant+ (2022a)] A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022).
[Dechant+(2022b)] A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022).
[SI (2023)] SI. Information Geometry, 1-42 (2023).

Related talks from my lab.

Talk by Kohei Yoshimura [T2b-07B-06]

[Yoshimura+ (2023)] K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023).
[Kolchinsky+ (2022)] A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).
[Yoshimura&SI (2023)] K. Yoshimura and SI. arXiv:2305.19519 (2023).

Talk by Naruo Ohga [T2b-07B-02]

[Ohga&SI (2022)] N. Ohga and SI. Phys. Rev. E **106**, 044131 (2022).
[Ohga&SI (2021)] N. Ohga and SI. arXiv:2112.11008 (2021).

Talk by Ryuna Nagayama [T2-08B-05]

[Hoshino+ (2023)] M. Hoshino, R. Nagayama, K. Yoshimura, JF Yamagishi and SI. Phys. Rev. Res. 5, 023127 (2023).

THE UNIVERSITY OF TOKYO

SCHOOL OF SCIENCE THE UNIVERSITY OF TOKYO

Universal Biology Institute

Our studies on geometric thermodynamics and related topics

Stochastic thermodynamics for Fokker-Planck equation / Langevin equation

Trade-offs [SI&Dechant (2020)], Minimum entropy production [Nakazato&SI (2021)], Decomposition (housekeeping/excess) [Dechant+ (2022a,b)], Concept of geometric thermodynamics [SI (2023)]

[SI&Dechant (2020)] SI and A. Dechant. Phys. Rev. X **10**, 021056 (2020). [Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021). [Dechant+ (2022a)] A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022). [Dechant+(2022b)] A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022). [SI (2023)] SI. Information Geometry, 1-42 (2023).

Stochastic thermodynamics for the master equation / Markov jump process

Speed limit [SI (2018)], Decomposition (Information thermodynamics) [SI+ (2020)], TURs and estimation of EPR [Otsubo+ (2020)], Duality [Ohga&SI (2021)], Information-thermodynamic minimum entropy production [Fujimoto&SI (2021)] Stability [SI (2022)], TURs [Kamijima+ (2023)], Bounds on cross-correlations [Ohga+ (2023)], Bounds on spectral perturbation [Kolchinsky+ (2023)]

[SI (2018)] SI. Phys. Rev. Lett. **121**, 030605 (2018). [SI+ (2020)] SI, M. Oizumi and S-I Amari. Phys. Rev. Res. **2**, 033048 (2020). [Otsubo+ (2020)] S. Otsubo, SI, A. Dechant and T. Sagawa. Phys. Rev. E. **101**, 062106 (2020). [Ohga&SI (2021)] N. Ohga and SI. arXiv: 2112.11008 (2021). [Fujimoto&SI (2021)] Y. Fujimoto and SI. arXiv: 2112.14035 (2021). [SI (2022)] SI. J. Phys. A. **55**, 054001 (2022). [Kamijima+ (2023)] T. Kamijima, SI, A. Dechant and T. Sagawa. Phys. Rev. E. **107**, L052101 (2023). [Ohga+ (2023)] N. Ohga, SI and A. Kolchinsky.Phys. Rev. Lett. In press. (2023). [Kolchinsky+ (2023)] A. Kohchinsky, N. Ohga and SI arXiv:2303.13116 (2023).

Deterministic chemical thermodynamics for the rate equation / chemical reaction networks

Speed limit [Yoshimura&SI (2021a)], Biological experiment of speed limit [Ashida+ (2021)] TURs [Yoshimura&SI (2021b)], Duality [Ohga&SI (2022)], Decomposition (housekeeping/excess) [Yoshimura+ (2023), Kolchinsky+ (2022)]

[Yoshimura&SI (2021a)] K. Yoshimura and SI. Phys. Rev. Res. **3**, 013175 (2021). [Ashida+ (2020)] K. Ashida, K. Aoki and SI. BioRxiv (2021). [Yoshimura&SI (2021b)] K. Yoshimura and SI. Phys. Rev. Lett. **127**, 160602 (2021). [Ohga&SI (2022)] N. Ohga and SI. Phys. Rev. E. **106**, 044131 (2022). [Yoshimura+ (2023)] K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023). [Kolchinsky+ (2022)] A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Evolutionary processes in population dynamics

Trade-offs [Hoshino+ (2023)]

[Hoshino+ (2023)] ≈

Macroscopic thermodynamics for Navier-Stokes equation

Decomposition (housekeeping/excess) [Yoshimura&SI (2023)]

[Yoshimura&SI (2023)] K. Yoshimura and SI, arXiv:2305.19519 (2023).

“Non-stochastic”

Geometric

~~Stochastic~~ thermodynamics

Our studies on geometric thermodynamics and related topics

Stochastic thermodynamics for Fokker-Planck equation / Langevin equation   Today's talk

Trade-offs [SI&Dechant (2020)], Minimum entropy production [Nakazato&SI (2021)], Decomposition (housekeeping/excess) [Dechant+ (2022a,b)], Concept of geometric thermodynamics [SI (2023)]

[SI&Dechant (2020)] SI and A. Dechant. Phys. Rev. X **10**, 021056 (2020). [Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021). [Dechant+ (2022a)] A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022). [Dechant+(2022b)] A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022). [SI (2023)] SI. Information Geometry, 1-42 (2023).

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Evolutionary processes in population dynamics

Trade-offs [Hoshino+ (2023)]

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Macroscopic thermodynamics for Navier-Stokes equation

Decomposition (housekeeping/excess) [Yoshimura&SI (2023)]

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"Non-stochastic"

Geometric ~~Stochastic~~ thermodynamics

Geometric thermodynamics

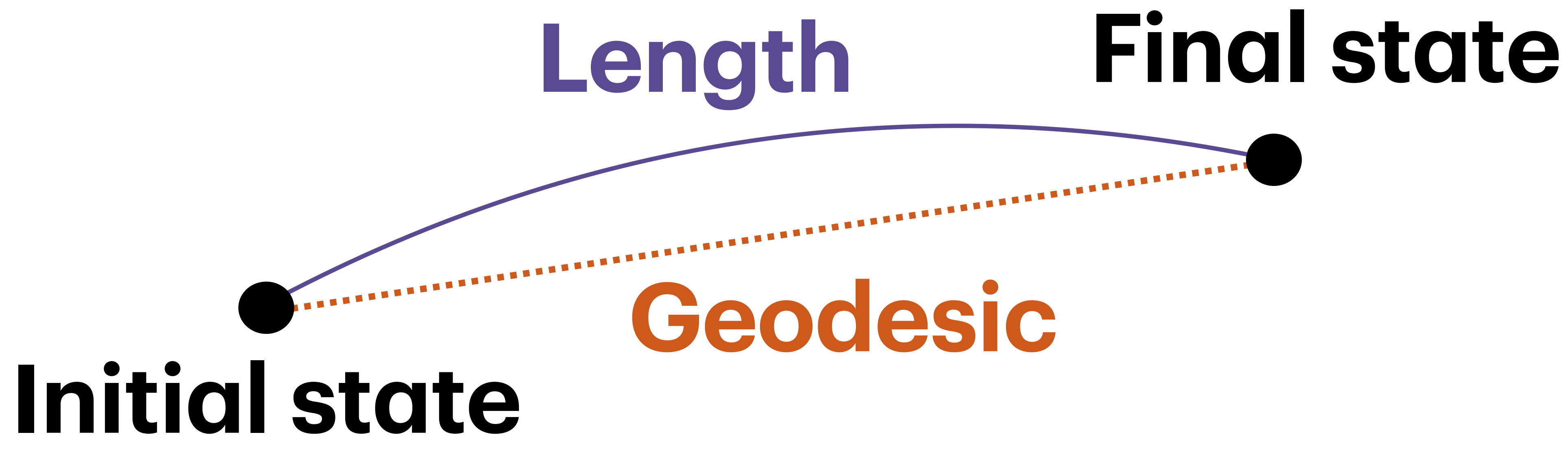
A theory of nonequilibrium thermodynamics based on (differential) geometry

Based on (differential) geometry, we can discuss ...

① a nonequilibrium transition characterized by the length

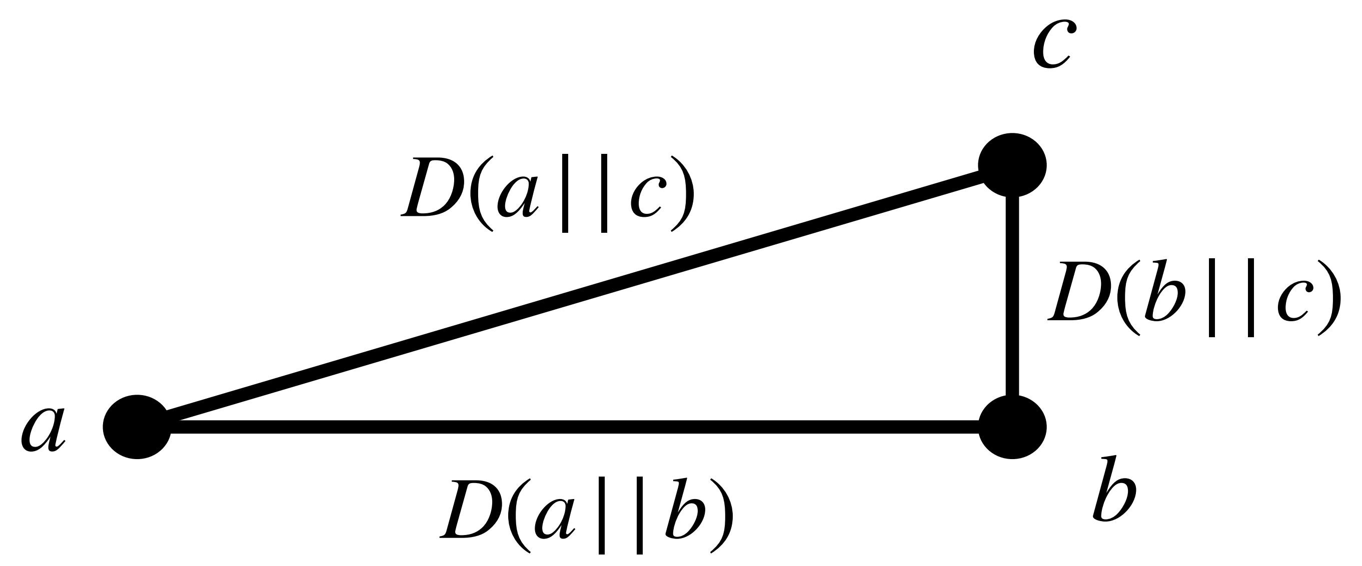
and its optimality characterized by geodesic

e.g.,) Minimum entropy production, Speed limit



② decompositions of thermodynamic cost via the orthogonality

e.g.,) Excess/housekeeping EPR, Information thermodynamics

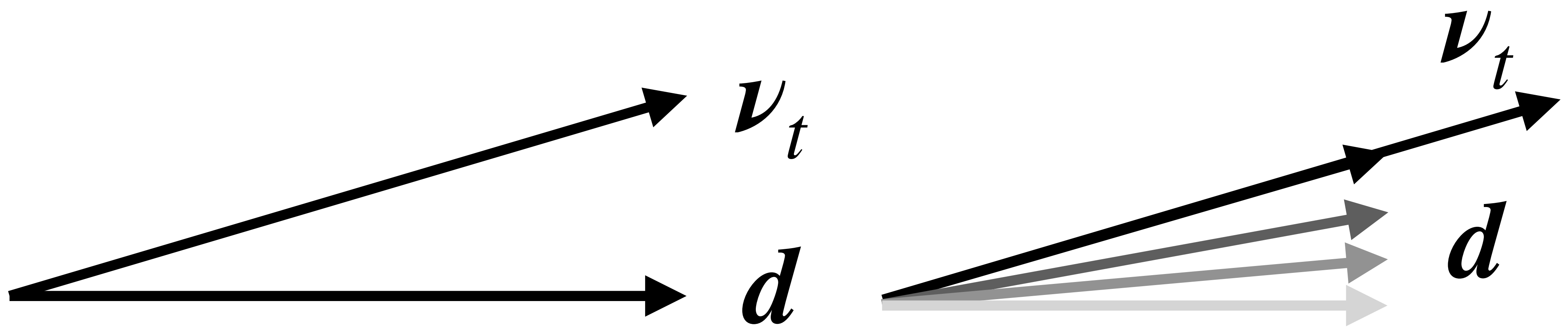


$D(a||c) = D(a||b) + D(b||c)$

③ thermodynamic trade-off relations based on the inner product

e.g.,) Thermodynamic uncertainty relations (TURs),

Estimation of entropy production rate (EPR)



$\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2 \leq \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle \langle \boldsymbol{d}, \boldsymbol{d} \rangle$

$\langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle = \max_{\boldsymbol{d}} \frac{\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle}$

④ duality, ⑤ stability, ⑥ perturbation ...etc.

Fokker-Planck equation and stochastic thermodynamics

Fokker-Planck equation

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x})) \qquad \boldsymbol{\nu}_t(\boldsymbol{x}) = \mu \boldsymbol{F}_t(\boldsymbol{x}) - \mu T \nabla \ln P_t(\boldsymbol{x})$$

Entropy production rate (EPR)

$$\sigma_t = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x}) = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle \; (\geq 0)$$

The 2nd law

Inner product (geometric):

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle = \frac{1}{\mu T} \int d\boldsymbol{x} [\boldsymbol{a}(\boldsymbol{x}) \cdot \boldsymbol{b}(\boldsymbol{x})] P_t(\boldsymbol{x})$$

EPR with the detailed balance condition $\boldsymbol{F}_t(\boldsymbol{x}) = -\nabla U(\boldsymbol{x}) = T \nabla \ln P^{\mathrm{eq}}(\boldsymbol{x})$

$$\sigma_t = \langle \mu T \nabla \ln P_t / P^{\mathrm{eq}}, \mu T \nabla \ln P_t / P^{\mathrm{eq}} \rangle = -\partial_t D_{\mathrm{KL}}(P_t \| P^{\mathrm{eq}})$$

Fokker-Planck Eq.: $\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot \left[\mu T P_t(\boldsymbol{x}) \nabla \ln \frac{P_t(\boldsymbol{x})}{P^{\mathrm{eq}}(\boldsymbol{x})} \right]$

Kullback-Leibler divergence (geometric):

$$D_{\mathrm{KL}}(P_t \| P^{\mathrm{eq}}) = \int d\boldsymbol{x} P_t(\boldsymbol{x}) \ln \frac{P_t(\boldsymbol{x})}{P^{\mathrm{eq}}(\boldsymbol{x})}$$

The 2nd law: $\partial_t D_{\mathrm{KL}}(P_t \| P^{\mathrm{eq}}) \leq 0$ ➡ $D_{\mathrm{KL}}(P_t \| P^{\mathrm{eq}})$:Lyapunov function $P_t \to P^{\mathrm{eq}}$ $(t \to \infty)$

Optimal transport theory and minimum entropy production

Optimal transport theory (Benamou-Brenier formula) [Benamou&Brenier (2000)]

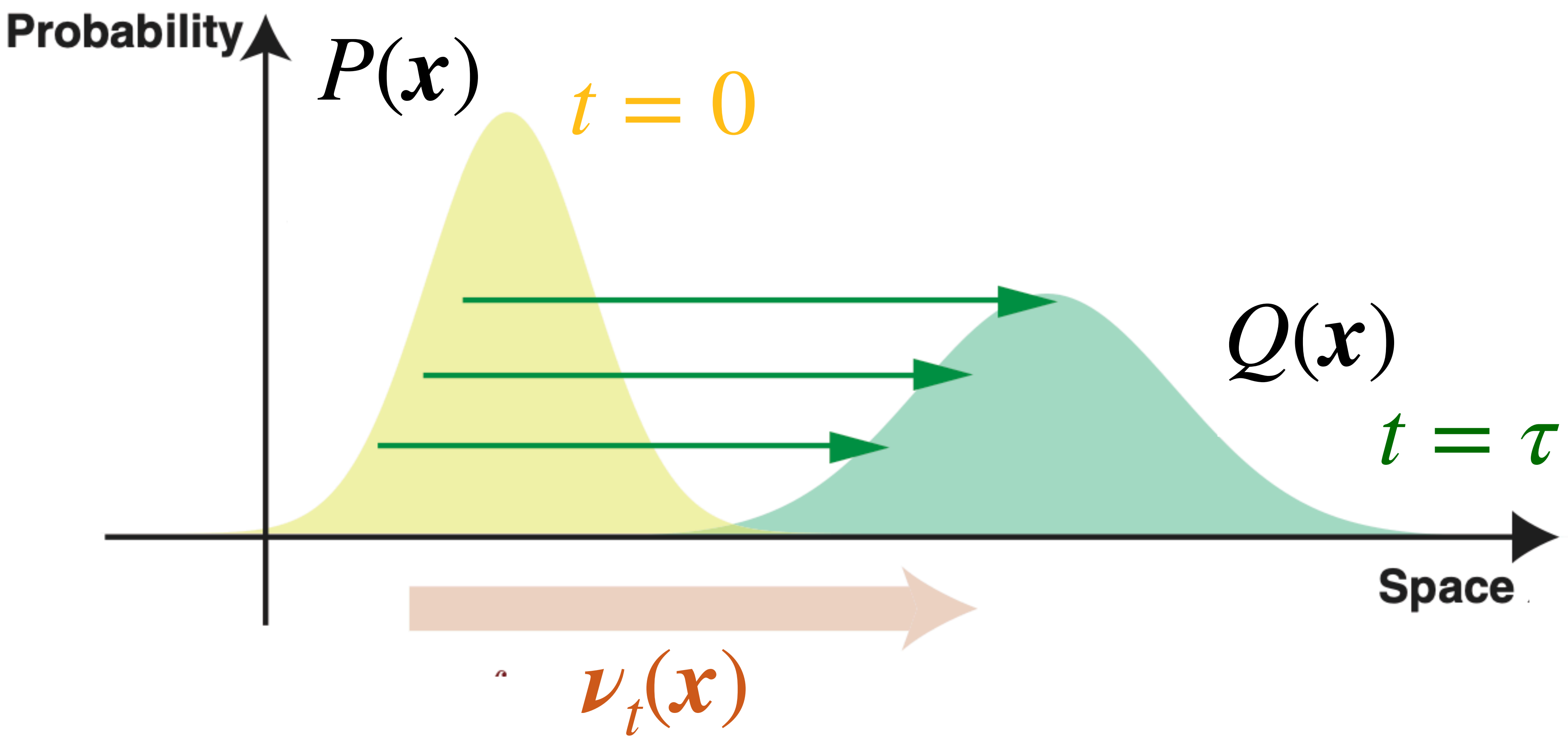
[Benamou&Brenier (2000)] J. D. Benamou and Y. Brenier. Numerische Mathematik, **84**, 375-393 (2000).

L^2-Wasserstein distance (geometric):

$$\mathcal{W}_2(P,Q) = \sqrt{\min_{(\boldsymbol{\nu}_t(\boldsymbol{x}),P_t(\boldsymbol{x}))_{0\le t\le\tau}} \tau \int_0^\tau dt \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x})}$$

$$\text{s.t.} \quad \partial_t P_t(\boldsymbol{x}) = -\nabla\cdot(\boldsymbol{\nu}_t(\boldsymbol{x})P_t(\boldsymbol{x}))$$

$$P_0(\boldsymbol{x}) = P(\boldsymbol{x}),\, P_\tau(\boldsymbol{x}) = Q(\boldsymbol{x})$$



Optimal $\boldsymbol{\nu}_t$:

$$\mathcal{W}_2(P,Q) = \sqrt{\tau \int_0^\tau dt \int d\boldsymbol{x} \|\nabla\Phi_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x})}$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \nabla\Phi_t(\boldsymbol{x}) \qquad \partial_t\Phi_t(\boldsymbol{x}) + \frac{1}{2}\|\nabla\Phi_t(\boldsymbol{x})\|^2 = 0$$

Minimum entropy production [Aurell+ (2011,2012)]

$$\Sigma_\tau = \int_0^\tau dt \sigma_t \ge \frac{[\mathcal{W}_2(P_0,P_\tau)]^2}{\mu T \tau}$$

[Aurell+ (2011)] E. Aurell, E., C. Mejía-Monasterio and P. Muratore-Ginanneschi. Phys. Rev. Lett. **106**, 250601 (2011).
[Aurell+ (2012)] E. Aurell, K. Gawędzki, C. Mejía-Monasterio, R. Mohayaee and P. Muratore-Ginanneschi. J. Stat. Phys. **147**, 487 (2012).

Geometric interpretation of nonequilibrium transition

[Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).
[SI (2023)] SI. Information geometry, 1-42 (2023).

Lower bound on EPR

$$\sigma_t \geq \frac{1}{\mu T}\left(\frac{d\mathscr{L}_t}{dt}\right)^2 = \langle \nabla \phi_t, \nabla \phi_t \rangle := \sigma_t^{\mathrm{ex}}$$

Excess EPR

Speed in L²-Wasserstein space (Geometric):

$$\frac{d\mathscr{L}_t}{dt} = \lim_{\Delta t \to 0} \frac{[\mathscr{W}_2(P_t, P_{t+\Delta t})]}{\Delta t}$$

Same time evolution by the "potential" $\phi_t(\boldsymbol{x})$: $\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x})) = -\nabla \cdot (\nabla \phi_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$

Minimum entropy production (thermodynamic speed limit)

$$\Sigma_t \geq \int_0^\tau dt \sigma_t^{\mathrm{ex}} \geq \frac{[\mathscr{L}_\tau - \mathscr{L}_0]^2}{\mu T \tau} \geq \frac{[\mathscr{W}_2(P_0, P_\tau)]^2}{\mu T \tau}$$

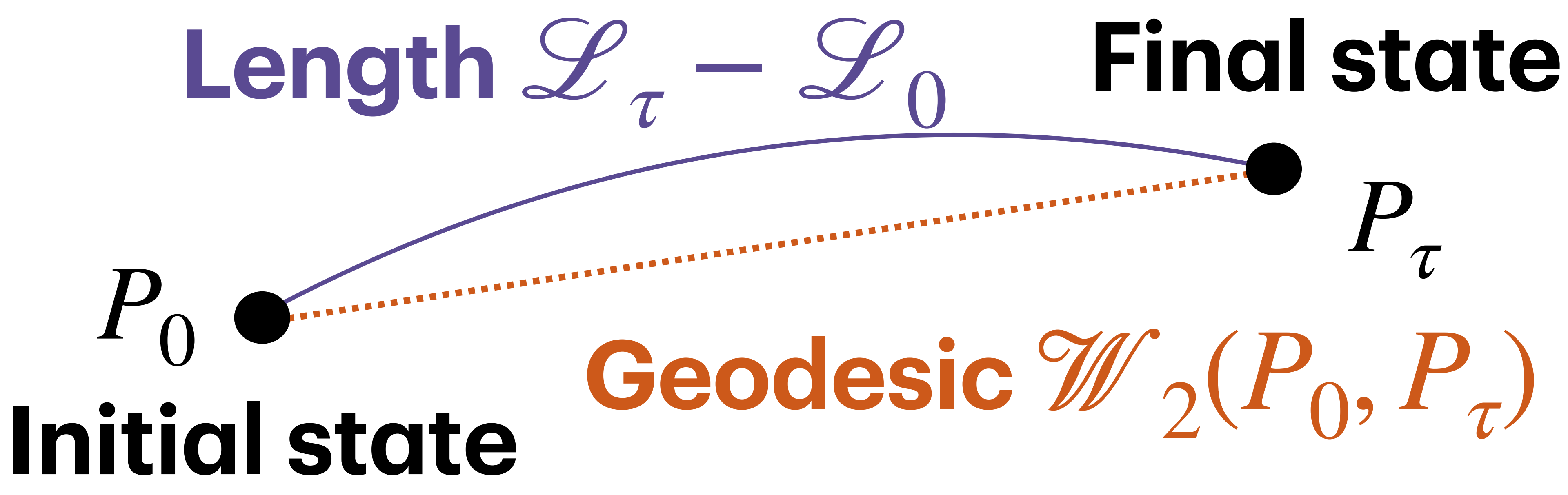
Optimal protocol (geodesic ∩ dynamics driven by potential)

$$\frac{d\mathscr{L}_t}{dt} = \frac{\mathscr{W}_2(P_0, P_\tau)}{\tau} = \mathrm{const}.$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \nabla \phi_t(\boldsymbol{x})$$

→

$$\Sigma_t = \frac{[\mathscr{W}_2(P_0, P_\tau)]^2}{\mu T \tau}$$



Example: Optimal protocol

[Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).

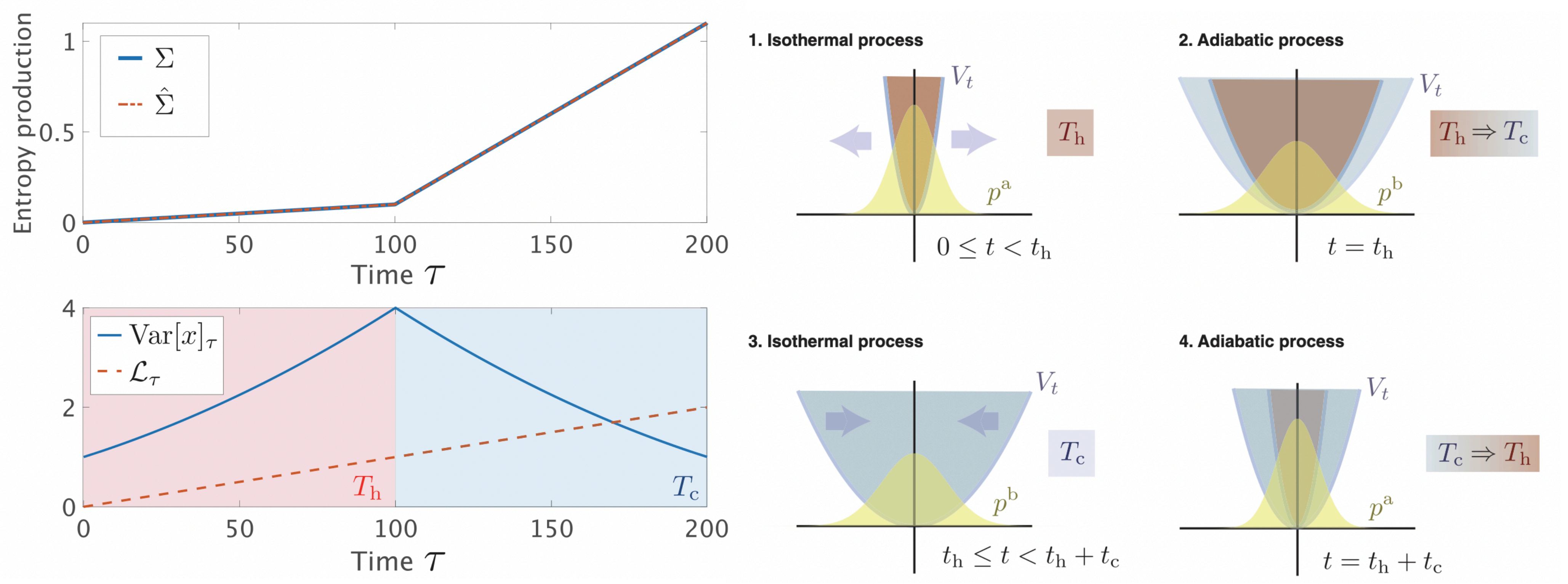
Harmonic potential, 1D Gaussian ($\boldsymbol{x} = x \in \mathbb{R}^1$)

$$\partial_t P_t(x) = -\partial_x(\nu_t(x)P_t(x)) \quad \nu_t(x) = \mu F_t(x) - \mu T \partial_x \ln P_t(x)$$

$$F_t(x) = -\partial_x U(x) = -k_t(x - a_t)$$

$$P_t(x) = \frac{1}{\sqrt{2\pi \mathrm{Var}[x]_t}} \exp\left(-\frac{(x - \mathbb{E}[x]_t)^2}{2\mathrm{Var}[x]_t}\right)$$

e.g.,) Optimal heat engine $\left(\frac{d\mathscr{L}_t}{dt} = \mathrm{const}.\right)$



L²-Wasserstein distance (1D Gaussian):

$$\mathscr{W}_2(P_s, P_t) = \sqrt{(\mathbb{E}[x]_s - \mathbb{E}[x]_t)^2 + (\sqrt{\mathrm{Var}[x]_s} - \sqrt{\mathrm{Var}[x]_t})^2}$$

Optimal protocol (Minimum dissipation in a finite time τ)

$$\frac{d\mathscr{L}_t}{dt} = \frac{\mathscr{W}_2(P_0, P_\tau)}{\tau} = \mathrm{const}.$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \nabla \phi_t(\boldsymbol{x})$$

→

$$\frac{d\mathbb{E}[x]_t}{dt} = \mathrm{const}.$$

$$\frac{d\sqrt{\mathrm{Var}[x]_t}}{dt} = \mathrm{const}.$$

→

$$a_t = \mathbb{E}[x]_t + \frac{\mathbb{E}[x]_\tau - \mathbb{E}[x]_0}{k_t \mu \tau}$$

$$k_t = \frac{T}{\mathrm{Var}[x]_t} - \frac{\sqrt{\mathrm{Var}[x]_\tau} - \sqrt{\mathrm{Var}[x]_0}}{\mu\tau\sqrt{\mathrm{Var}[x]_t}}$$

Geometric excess/housekeeping decomposition of EPR

[Nakazato&SI (2021)] M. Nakazato and SI. Phys. Rev. Res. **3**, 043093 (2021).
[Dechant+ (2022a)] A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022).

Geometric decomposition

$$\sigma_t = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle = \underbrace{\langle \nabla \phi_t, \nabla \phi_t \rangle}_{:= \sigma_t^{\mathrm{ex}}} + \underbrace{\langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{\nu}_t - \nabla \phi_t \rangle}_{:= \sigma_t^{\mathrm{hk}}}$$

σ_t^{hk} is same as σ_t^{rot} in [Nakazato&SI (2021)].

σ_t^{ex} :Excess EPR

(The dissipation by the same time evolution driven by a potential)

$$\nabla \phi_t(\boldsymbol{x}) \in \mathrm{Im}[\mathrm{grad}]$$

σ_t^{hk} :Housekeeping EPR

(The dissipation by cycle flows which do not affect the time evolution)

$$[\boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla \phi_t(\boldsymbol{x})]P_t(\boldsymbol{x}) \in \mathrm{Ker}[-\mathrm{div}]$$

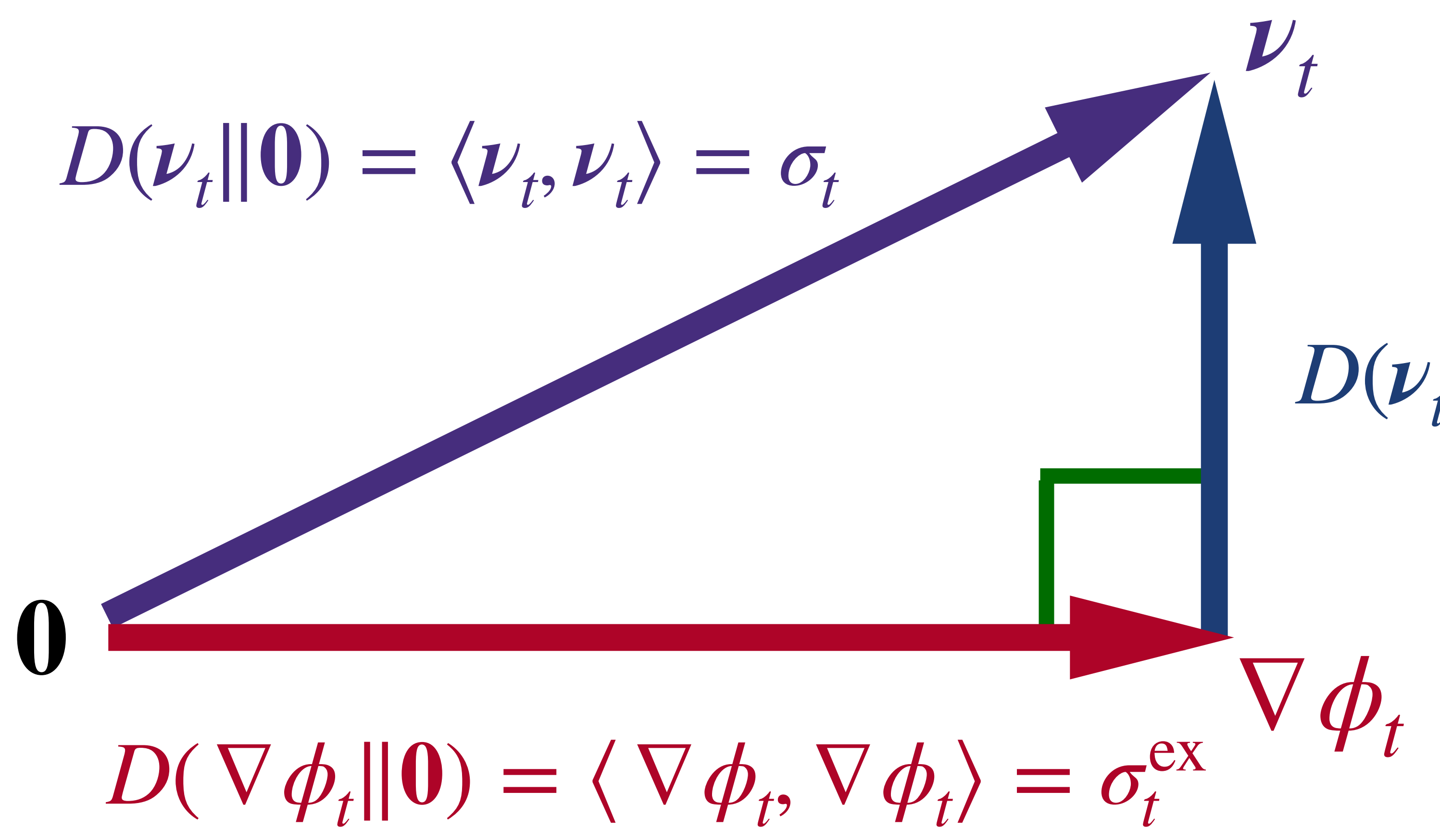
$$-\nabla \cdot ([\boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla \phi_t(\boldsymbol{x})]P_t(\boldsymbol{x})) = 0$$

A same decomposition is introduced via $\nabla \cdot J^V = 0$ [Maes&Netočný (2014)].

[Maes&Netočný (2014)] C. Maes and K. Netočný. J. Stat. Phys. **154**, 188 (2014).

Pythagorean theorem

$$D(\boldsymbol{\nu}_t \| \mathbf{0}) = D(\boldsymbol{\nu}_t \| \nabla \phi_t) + D(\nabla \phi_t \| \mathbf{0})$$



$D(\boldsymbol{\nu}_t \| \nabla \phi_t) = \langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{\nu}_t - \nabla \phi_t \rangle = \sigma_t^{\mathrm{hk}}$

$\mathrm{Ker}[-\mathrm{div}] \perp \mathrm{Im}[\mathrm{grad}]$

Orthogonality: $\langle \boldsymbol{\nu}_t - \nabla \phi_t, \nabla \phi_t \rangle = 0$

Short-time TURs for excess/housekeeping EPR

[Dechant+ (2022a)] A. Dechant, S-I Sasa and SI. Phys. Rev. Res. **4**, L012034 (2022).
[Dechant+ (2022b)] A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022).

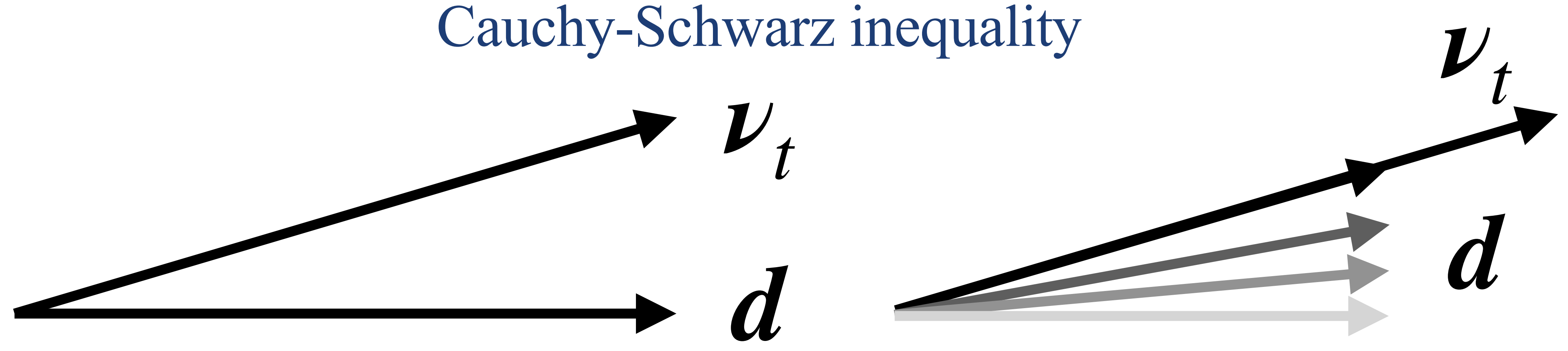
Short-time TUR for EPR

$$\sigma_t = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle \geq \frac{\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle} \qquad \sigma_t = \max_{\boldsymbol{d}} \frac{\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle}$$

Estimation of EPR by machine learning [Otsubo+ (2020)]

[Otsubo+ (2020)] S. Otsubo, SI, A. Dechant and T. Sagawa. Phys. Rev. E. **101**, 062106 (2020).

Cauchy-Schwarz inequality



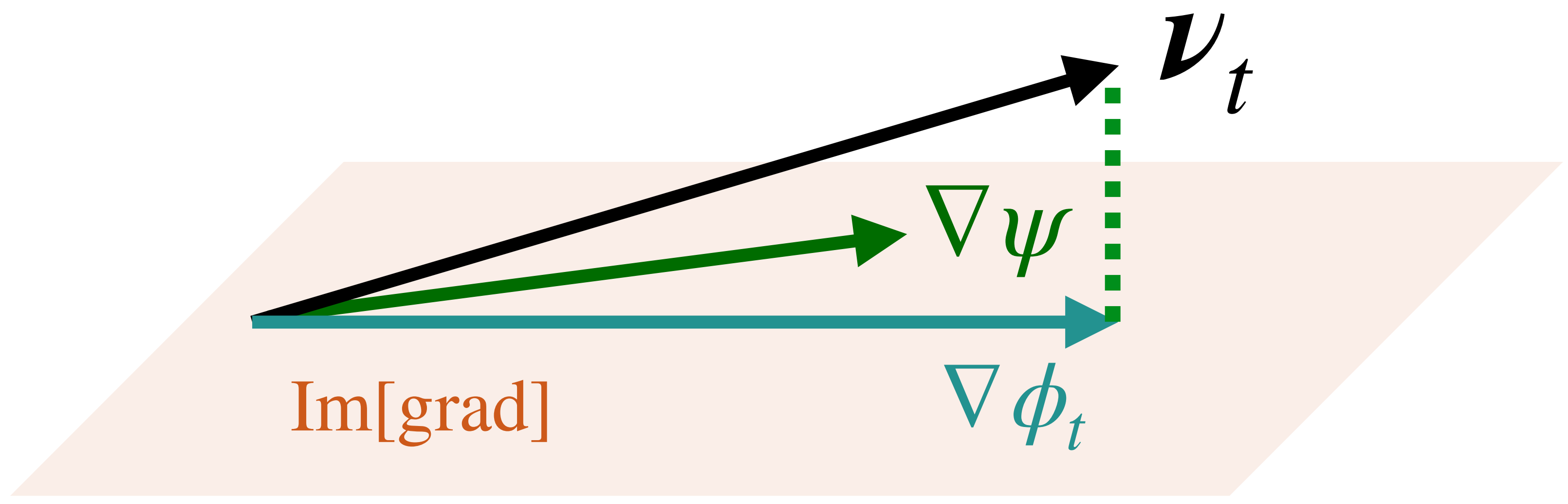
$$\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2 \leq \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle \langle \boldsymbol{d}, \boldsymbol{d} \rangle \qquad \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle = \max_{\boldsymbol{d}} \frac{\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle}$$

Short-time TUR for excess EPR

$$\sigma_t^{\mathrm{ex}} = \langle \nabla \phi_t, \nabla \phi_t \rangle \geq \frac{\langle \nabla \phi_t, \nabla \psi \rangle^2}{\langle \nabla \psi, \nabla \psi \rangle} = \frac{|\partial_t \mathbb{E}_t[\psi]|^2}{\langle \nabla \psi, \nabla \psi \rangle}$$

$$\sigma_t^{\mathrm{ex}} = \max_{\psi} \frac{\langle \boldsymbol{\nu}_t, \nabla \psi \rangle^2}{\langle \nabla \psi, \nabla \psi \rangle} = \max_{\psi} \frac{|\partial_t \mathbb{E}_t[\psi]|^2}{\langle \nabla \psi, \nabla \psi \rangle}$$

Expected value: $\mathbb{E}_t[\psi] = \int d\boldsymbol{x} \psi(\boldsymbol{x}) P_t(\boldsymbol{x})$



Short-time TUR for housekeeping EPR

$$\sigma_t^{\mathrm{hk}} \geq \frac{\langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle} \qquad \sigma_t^{\mathrm{hk}} = \max_{\boldsymbol{d} | \nabla \cdot (\boldsymbol{d} P_t) = 0} \frac{\langle \boldsymbol{\nu}_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle}$$

Excess EPR and gradient flow

[Dechant+ (2022b)] A. Dechant, S-I Sasa and SI. Phys. Rev. E **106**, 024125 (2022).
[SI (2023)] SI. Information geometry, 1-42 (2023).

An expression of excess EPR

$$\sigma_t^{\rm ex} = -\partial_t D_{\rm KL}(P_t \| P_s^{\rm pcan})\Big|_{s=t}$$

$$\nabla \phi_t(\boldsymbol{x}) = \mu T \nabla \ln P_t(\boldsymbol{x}) - \mu T \nabla \ln \underline{P_s^{\rm pcan}(\boldsymbol{x})}$$ Pseudo canonical distribution

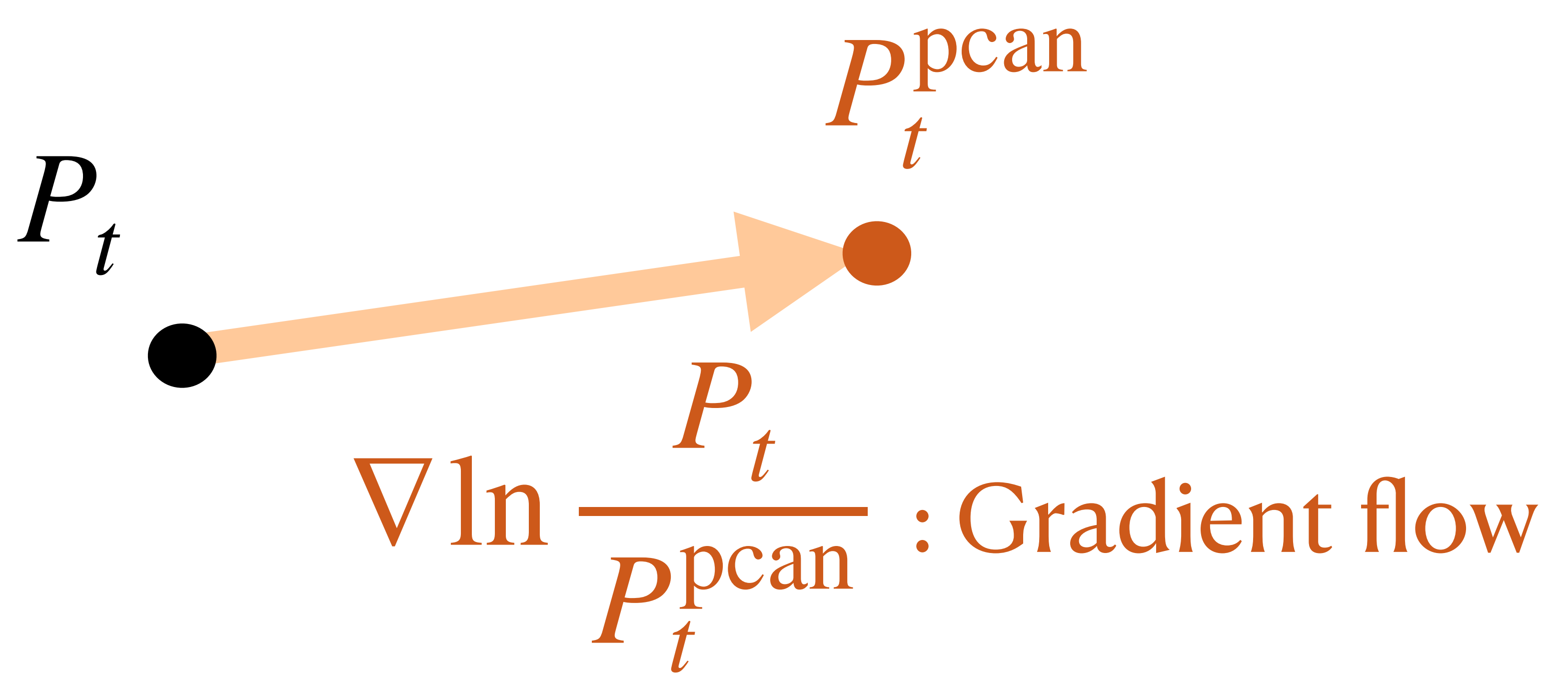
$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot [\nabla \phi_t(\boldsymbol{x}) P_t(\boldsymbol{x})] = -\nabla \cdot \left[\mu T P_t(\boldsymbol{x}) \underline{\nabla \ln \frac{P_t(\boldsymbol{x})}{P_t^{\rm pcan}(\boldsymbol{x})}} \right]$$

Gradient flow

cf.) EPR with the detailed balance condition

$$\sigma_t = -\partial_t D_{\rm KL}(P_t \| P^{\rm eq}) \; (\geq 0)$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu T \nabla \ln P_t(\boldsymbol{x}) - \mu T \nabla \ln P^{\rm eq}(\boldsymbol{x})$$



Non-negativity of excess EPR

$$\partial_t D_{\rm KL}(P_t \| P_s^{\rm pcan})\Big|_{s=t} \leq 0$$

$\partial_t P_t^{\rm pcan} = 0$ ⇒ A Lyapunov function exists. (Relaxation to a unique steady-state $P_t \to P_t^{\rm pcan}$ $(t \to \infty)$)

$P_t^{\rm pcan} = P_t^{\rm st}$ ⇒ The excess EPR $\sigma_t^{\rm ex}$ can be Hatano-Sasa excess (or non-adiabatic) EPR [Hatano&Sasa (2001), Esposito&Van den Broeck (2010)].

$\sigma_t^{\rm ex;HS} = -\partial_t D_{\rm KL}(P_t \| P_s^{\rm st})\Big|_{s=t}$. In general, $P_t^{\rm pcan} \neq P_t^{\rm st}$ and $\sigma_t^{\rm ex;HS} \leq \sigma_t^{\rm ex}$ [Dechant+ (2022b)].

[Hatano&Sasa (2001)] T. Hatano and S. I. Sasa, Physical review letters, **86**, 3463 (2001).
[Esposito&Van den Broeck (2001)] M. Esposito and C. Van den Broeck, Physical Review E, **82**, 011143 (2010).

Information-geometric orthogonality

[SI (2023)] SI. Information geometry, 1-42 (2023).
See also) [SI+ (2020)] SI, M. Oizumi and S-I Amari. Phys. Rev. Res. **2**, 033048 (2020). [Kolchinsky+ (2022)] A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Path probability for tilted dynamics:

$$\mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt}) = \mathbb{T}_{\boldsymbol{\nu}'}(\boldsymbol{x}_{t+dt} | \boldsymbol{x}_t) p_t(\boldsymbol{x}_t)$$

$$\mathbb{T}_{\boldsymbol{\nu}'}(\boldsymbol{x}_{t+dt} | \boldsymbol{x}_t) \propto \exp\left[- \frac{\| \boldsymbol{x}_{t+dt} - \boldsymbol{x}_t - (\mu \boldsymbol{F}_t(\boldsymbol{x}_t) + \boldsymbol{\nu}'(\boldsymbol{x}_t) - \boldsymbol{\nu}_t(\boldsymbol{x}_t)) dt \|^2}{4\mu T dt} \right]$$

Tilted dynamics:

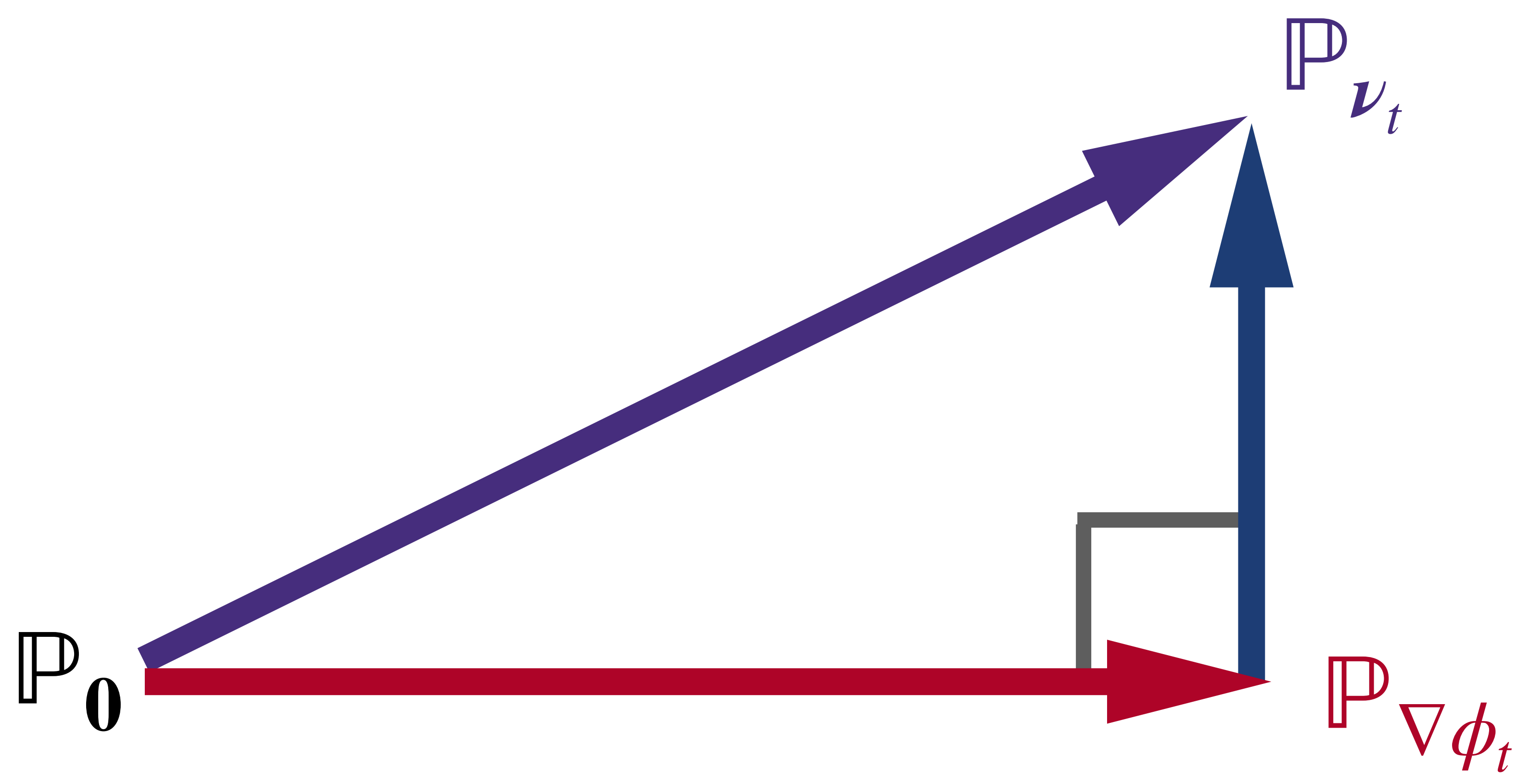
$$\partial_t p_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}(\boldsymbol{x}) + (\boldsymbol{\nu}'(\boldsymbol{x}) - \boldsymbol{\nu}(\boldsymbol{x})) p_t(\boldsymbol{x}))$$
$$= -\nabla \cdot (\boldsymbol{\nu}'(\boldsymbol{x}) p_t(\boldsymbol{x}))$$

Kullback-Leibler divergence (for two path probabilities):

$$D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}'} \| \mathbb{P}_{\boldsymbol{\nu}''}) = \int d\boldsymbol{x}_t d\boldsymbol{x}_{t+dt} \mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt}) \ln \frac{\mathbb{P}_{\boldsymbol{\nu}'}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt})}{\mathbb{P}_{\boldsymbol{\nu}''}(\boldsymbol{x}_t, \boldsymbol{x}_{t+dt})}$$

Generalized Pythagorean theorem (Information geometry)

$$\underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}_t} \| \mathbb{P}_{\mathbf{0}})}_{= \sigma_t dt/4} = \underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\boldsymbol{\nu}_t} \| \mathbb{P}_{\nabla \phi_t})}_{= \sigma_t^{\mathrm{hk}} dt/4} + \underbrace{D_{\mathrm{KL}}(\mathbb{P}_{\nabla \phi_t} \| \mathbb{P}_{\mathbf{0}})}_{= \sigma_t^{\mathrm{ex}} dt/4}$$



Two possible geometries of nonequilibrium thermodynamics

Information geometry

Differential geometry for the set of (path) probabilities

$$\{\mathbb{P}(z) \,|\, \mathbb{P}(z) \geq 0, \int dz \mathbb{P}(z) = 1\}$$

A geometric measure: Kullback-Leibler divergence

$$D_{\mathrm{KL}}(\mathbb{P} \| \mathbb{Q}) = \int dz \mathbb{P}(z) \ln \frac{\mathbb{P}(z)}{\mathbb{Q}(z)}$$

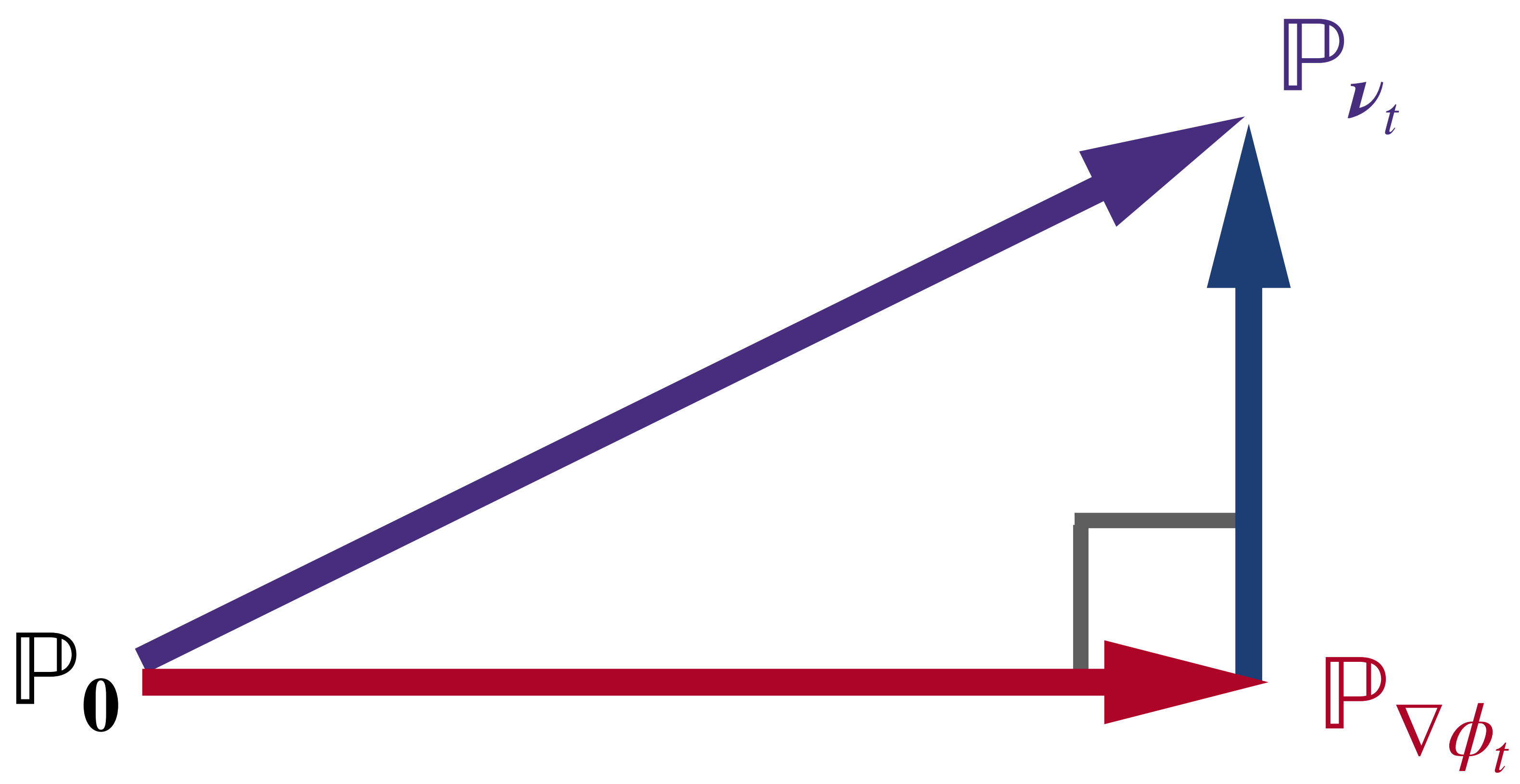
Optimal transport theory

Differential geometry for kinetics of $P_t(\boldsymbol{x})$

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x})) = -\nabla \cdot (\nabla \phi_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$$

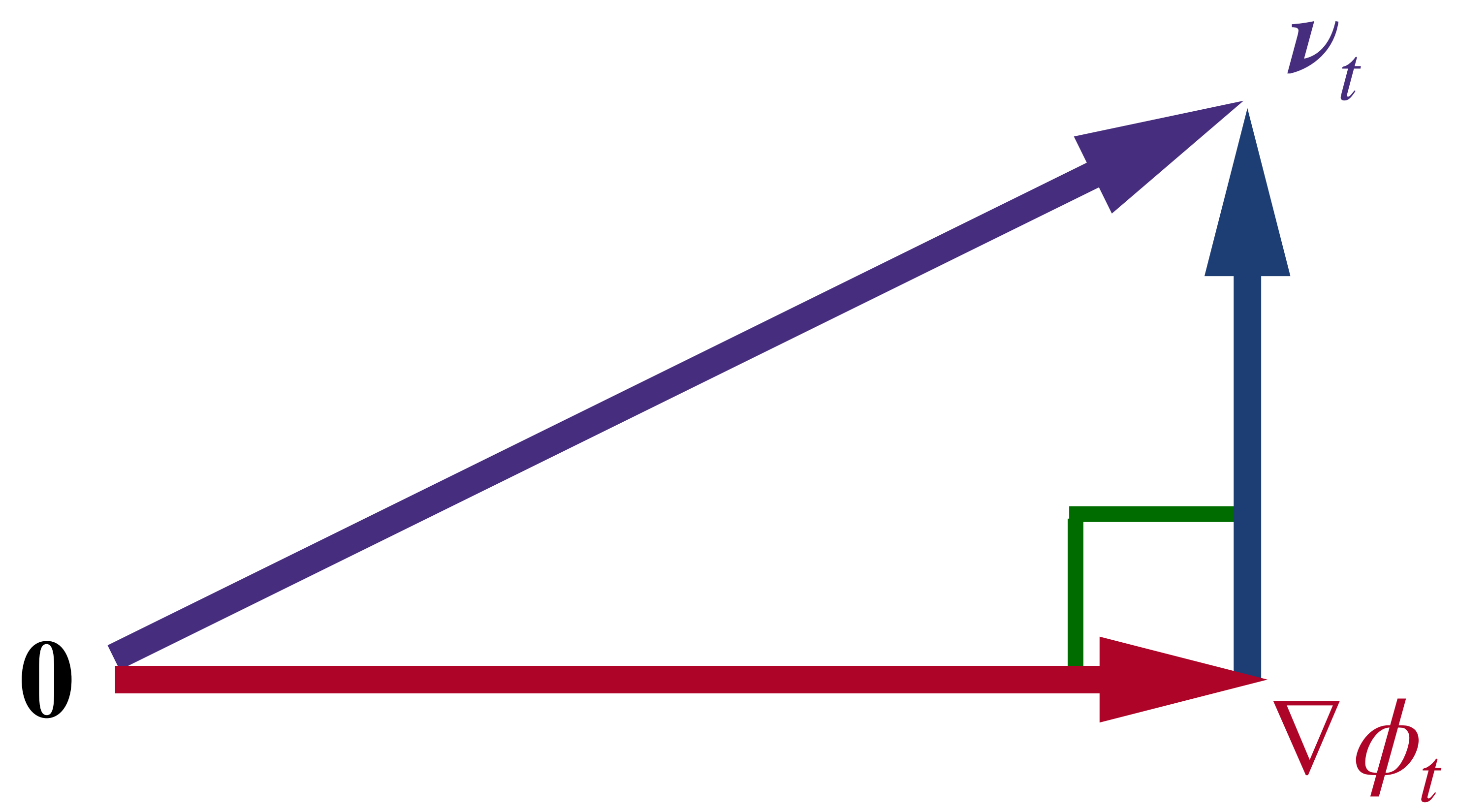
A geometric measure: L^2-Wasserstein divergence

$$\mathscr{W}_2(P_0, P_\tau) = \sqrt{\min_{\boldsymbol{\nu}_t} \tau \int_0^\tau dt \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x})} = \sqrt{\tau \int_0^\tau dt \langle \nabla \phi_t, \nabla \phi_t \rangle}$$



A decomposition of EPR

$$\sigma_t = \sigma_t^{\mathrm{ex}} + \sigma_t^{\mathrm{hk}}$$



Two geometries can provide different excess/housekeeping decompositions for the master/rate equation. [Yoshimura+ (2023), Kolchinsky+ (2022)]

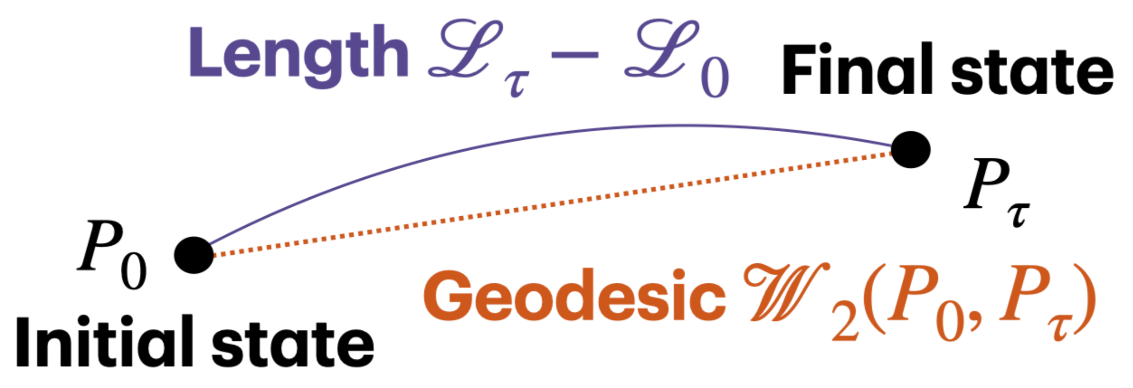
[Yoshimura+ (2023)] K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. **5**, 013017 (2023). [Kolchinsky+ (2022)] A. Kolchinsky, A. Dechant, K. Yoshimura and SI. arXiv:2206.14599 (2022).

Summary

We proposed a differential-geometric framework of nonequilibrium thermodynamics.

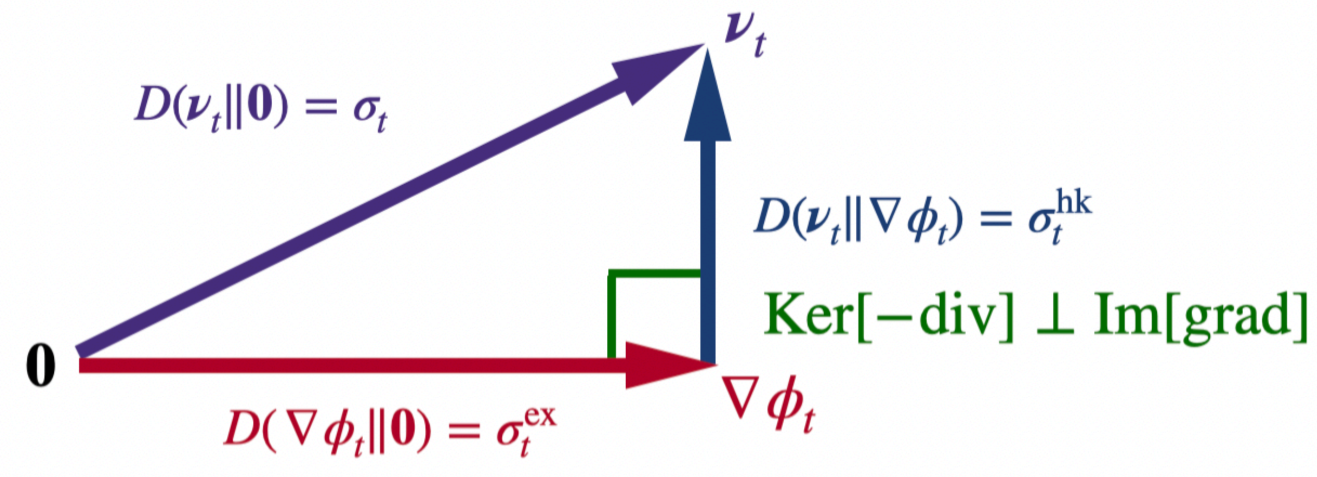
We can discuss minimum entropy production and optimal protocol based on geometry of optimal transport theory.

$$\Sigma_t \geq \int_0^\tau dt \sigma_t^{\mathrm{ex}} \geq \frac{[\mathscr{L}_\tau - \mathscr{L}_0]^2}{\mu T \tau} \geq \frac{[\mathscr{W}_2(P_0, P_\tau)]^2}{\mu T \tau}$$



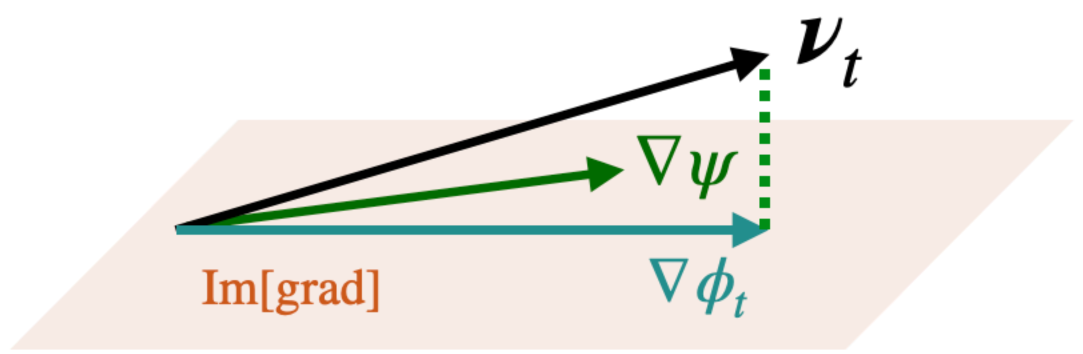
We obtained an excess/housekeeping decomposition of EPR via Pythagorean theorem.

$$\sigma_t = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle = \underbrace{\langle \nabla \phi_t, \nabla \phi_t \rangle}_{:= \sigma_t^{\mathrm{ex}}} + \underbrace{\langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{\nu}_t - \nabla \phi_t \rangle}_{= \sigma_t^{\mathrm{hk}}}$$



We obtained short-time TURs for excess/housekeeping EPR from an expression by an inner product.

$$\sigma_t^{\mathrm{ex}} \geq \frac{|\partial_t \mathbb{E}_t[\psi]|^2}{\langle \nabla \psi, \nabla \psi \rangle} \qquad \sigma_t^{\mathrm{hk}} \geq \frac{\langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{d} \rangle^2}{\langle \boldsymbol{d}, \boldsymbol{d} \rangle}$$



We revealed a thermodynamic link between geometry of Kullback-Leibler divergence in information geometry and geometry of L^2-Wasserstein distance in optimal transport theory for the Fokker-Planck equation.