Optimal transport theory as a geometric theory of non-equilibrium thermodynamics

StatPhys Seminar @UTokyoHongo

Sosuke Ito, Universal Biology Institute UTokyo, June 6th 2022.

M. Nakazato, and SI. *Physical Review Research* 3, 043093 (2021).
A. Dechant, S-I Sasa, and SI. *Physical Review Research* 4, L012034 (2022).
A. Dechant, S-I Sasa, and SI. *arXiv:2202.04331* (2022).
K. Yoshimura, A. Kolchinsky, A. Dechant, and SI. *arXiv:2205.15227* (2022). Submitted last week

生物普遍性研究機構
Universal Biology Institute

- **Lecture on optimal transport theory (within 30 mins)**
- **Geometric theory of non-equilibirum thermodynamics**

Introduction to optimal transport theory

A branch of mathematics about differential geometry, stochastic process, information theory and machine learning

- A lot of physical topics in the optimal transport theory

  Hamilton-Jacobi equation

  Gradient flow

  Eulerian/Lagrangian description

  Fokker-Planck equation

  Entropy

It seems to be physics of analytical mechanics, fluid dynamics, electromagnetism, and thermodynamics.

The old topic in economics

Two Nobel medals (Economics)

Leonid Kantorovich (1975)

Tjalling Koopmans (1975)

The new mainstream in mathematics

Two Fields medals in the 2010s

Cédric Villani (2010)

Alessio Figalli (2018)

My motivation

Based on optimal transport theory, I tried to construct a differential geometric theory of non-equilibrium thermodynamics which is well connected with mathematical framework of analytical mechanics, fluid dynamics and electromagnetism.

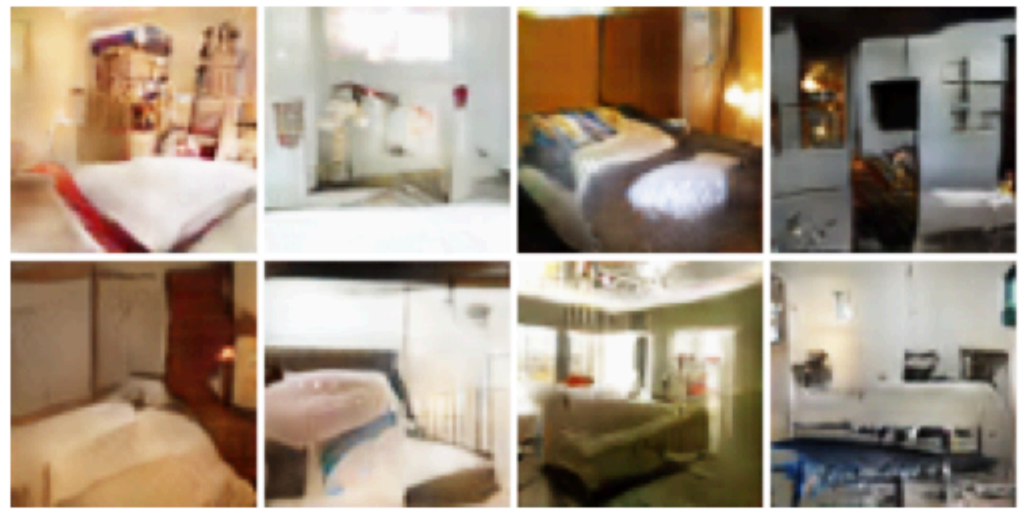
The trendy topic in machine learning

Conference on Neural Information Processing Systems

"Optimal Transport and Machine Learning" (Workshop series in '14, '17, '19, and '21)

Examples of optimal transport

Image generation (Wasserstein GAN)



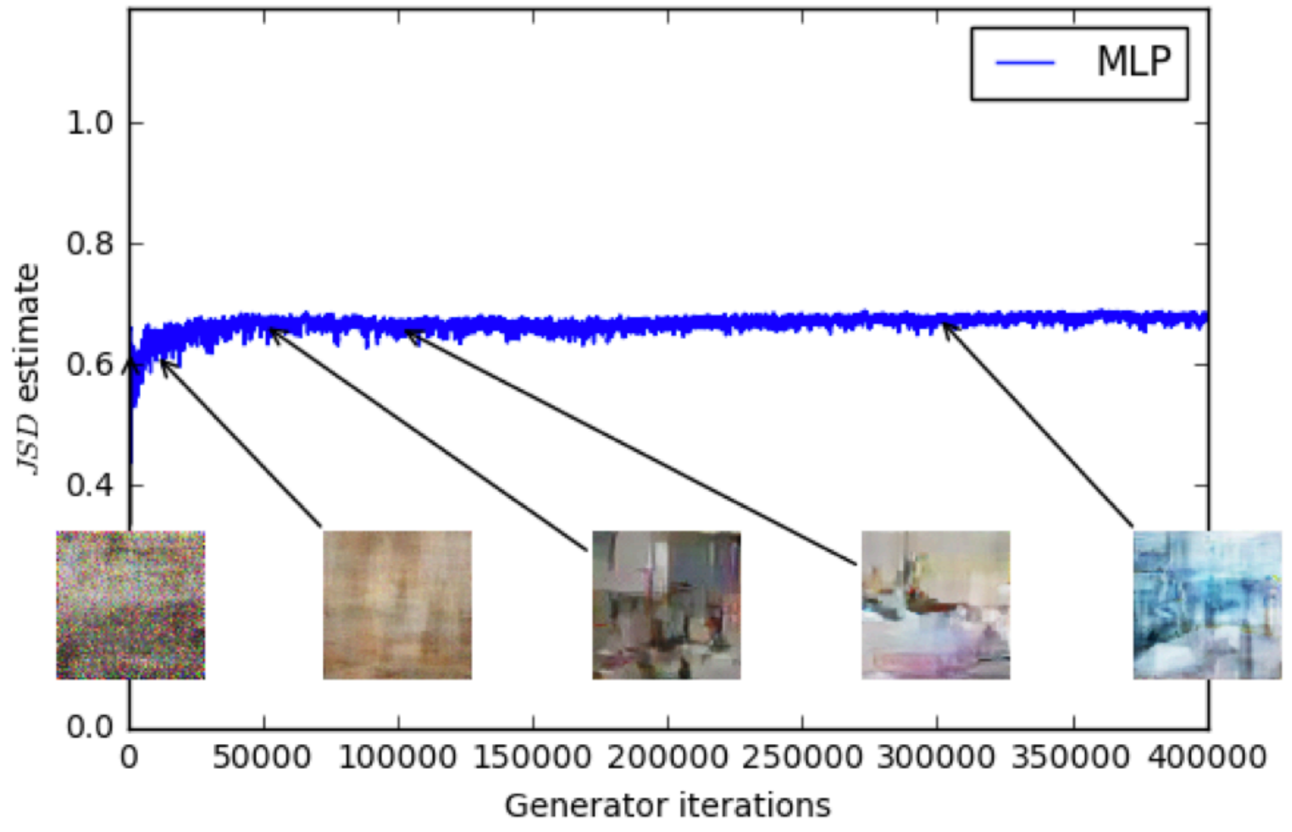


Image from learning

Arjovsky, Martin, et al. *International conference on machine learning*. PMLR, (2017).

Image interpolation (Benamou-Brenier algorithm)

Image 1

Image 2

Artificial images from optimal transport

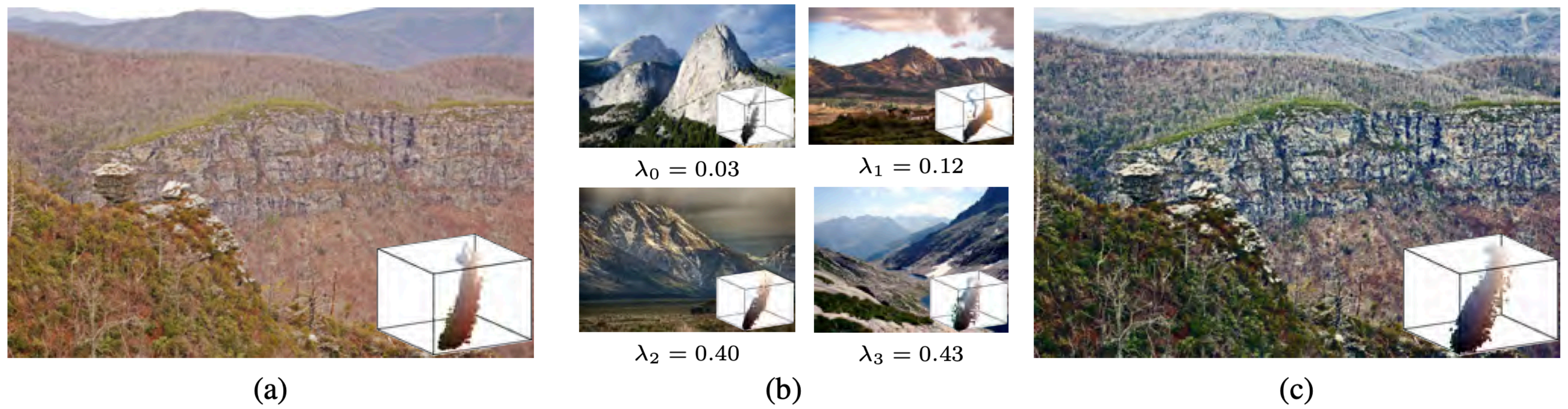
Lei Zhu, et al. IEEE trans on image processing, 16, 1481 (2007).

Color grading (Wasserstein Barycentric Coordinates)

Input1

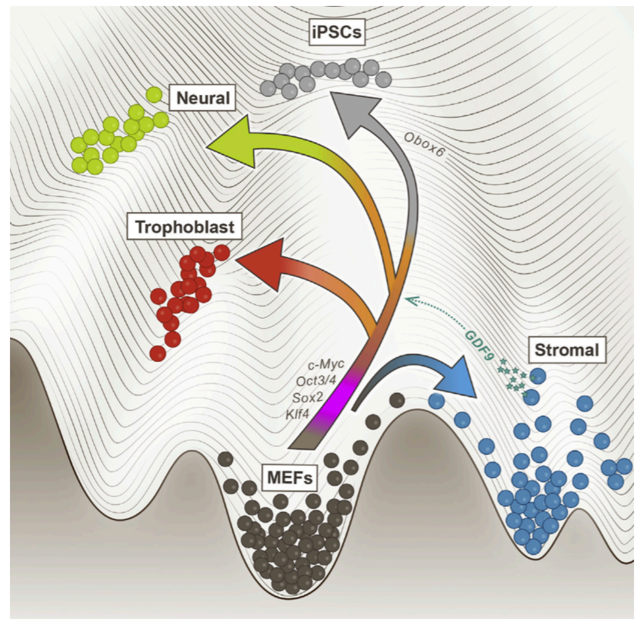
Input2

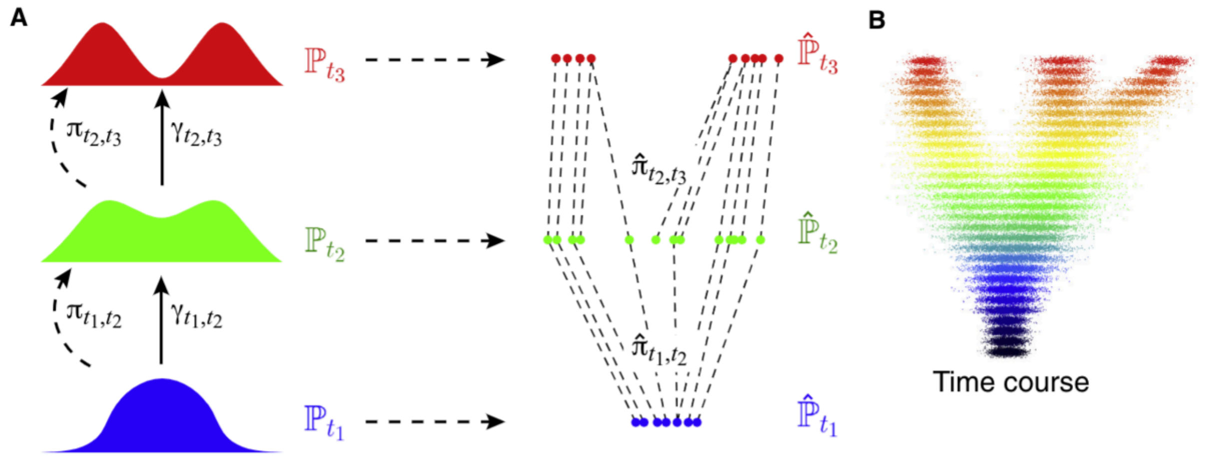
Output



Bonneel, Nicolas, et al. *ACM Trans. Graph.* 35, 71 (2016).

Analysis of cellular differentiation (Waddington-OT)





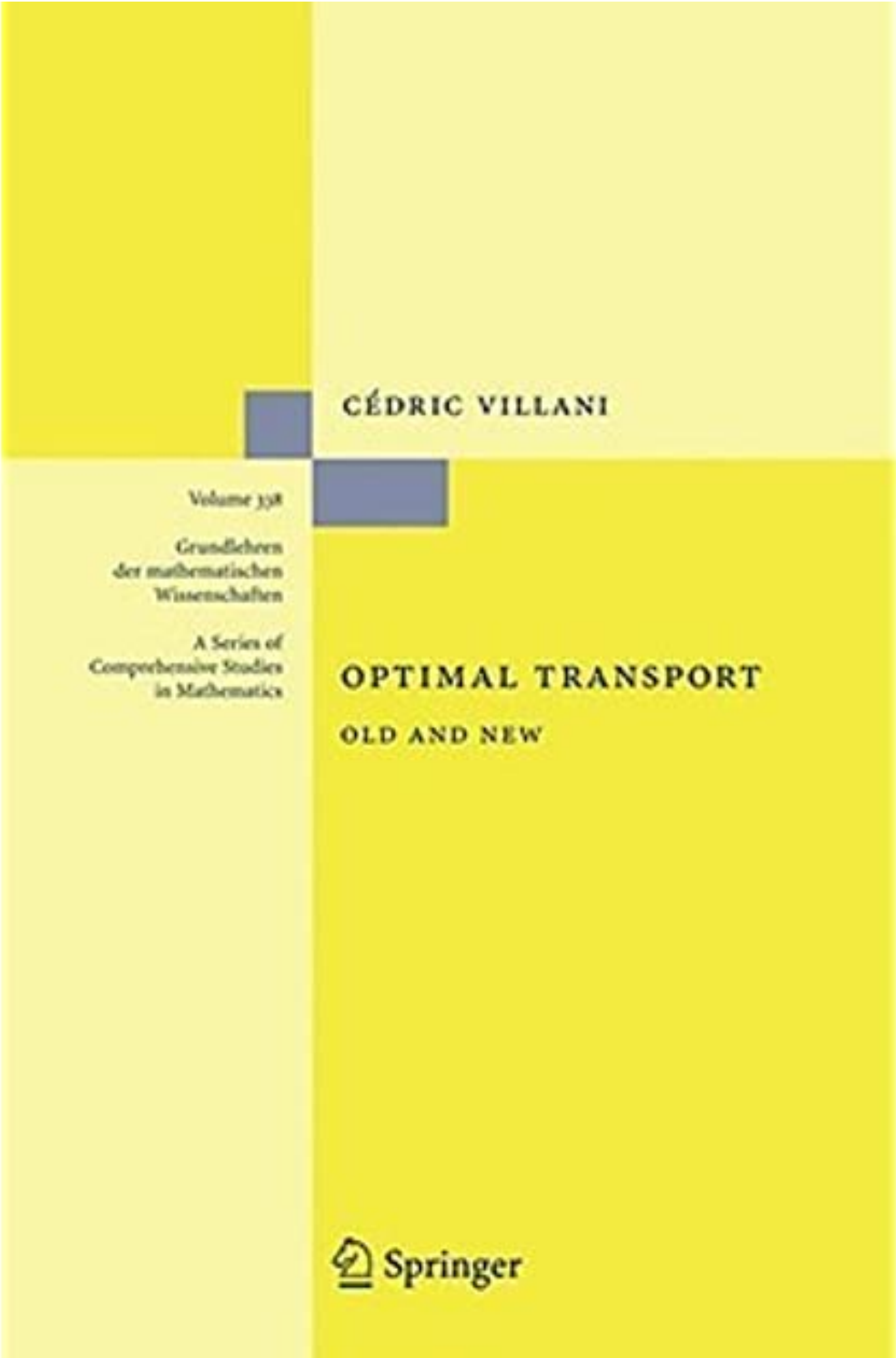
Waddington landscape

Schiebinger, Geoffrey, et al. *Cell* 176, 928-943 (2019).

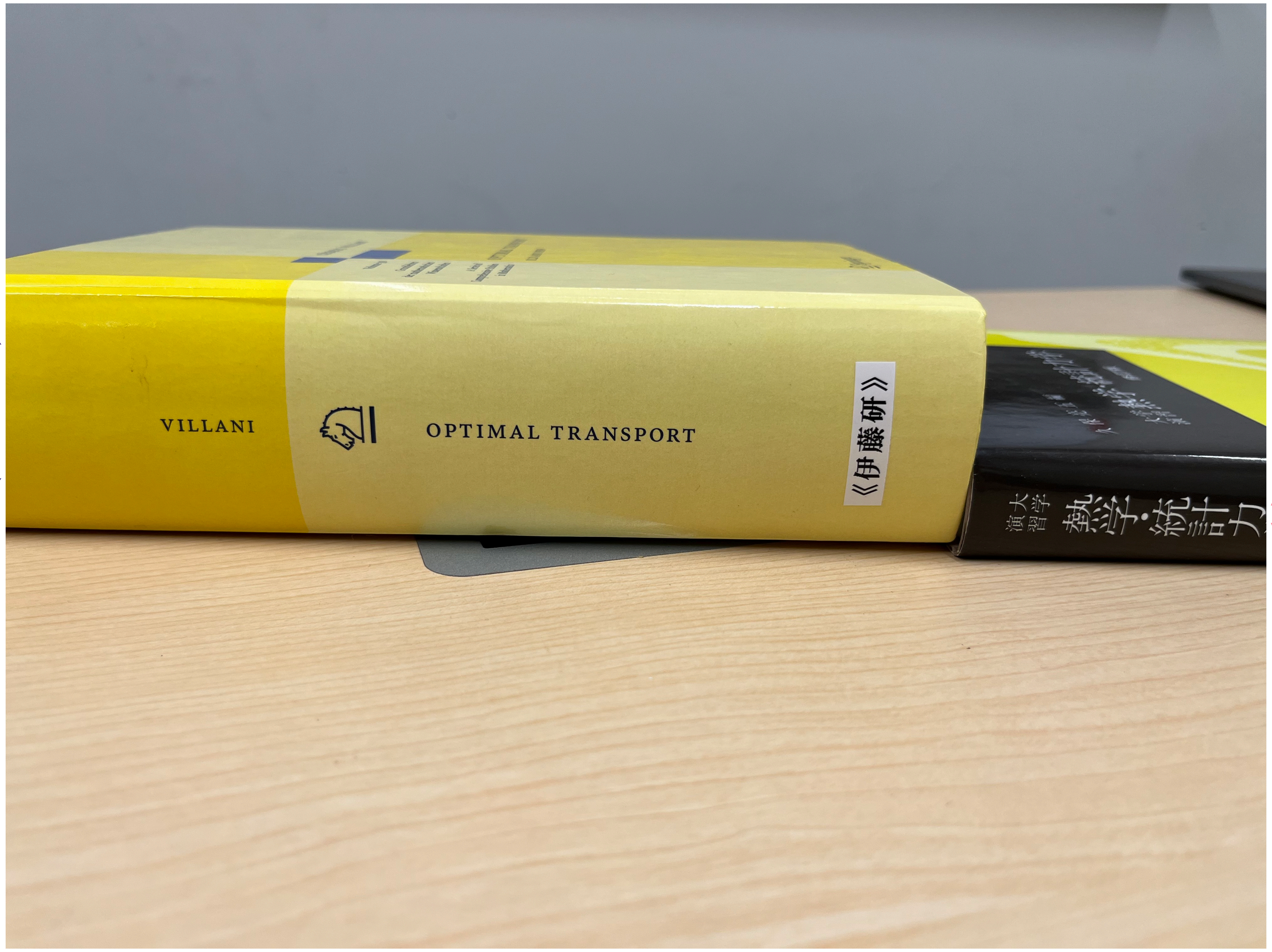
I would like to briefly introduce mathematics of optimal transport theory

Villani, C. (2009). *Optimal transport: old and new* (Vol. 338, p. 23). Berlin: springer.

within 30 mins...



~ 1000 pages



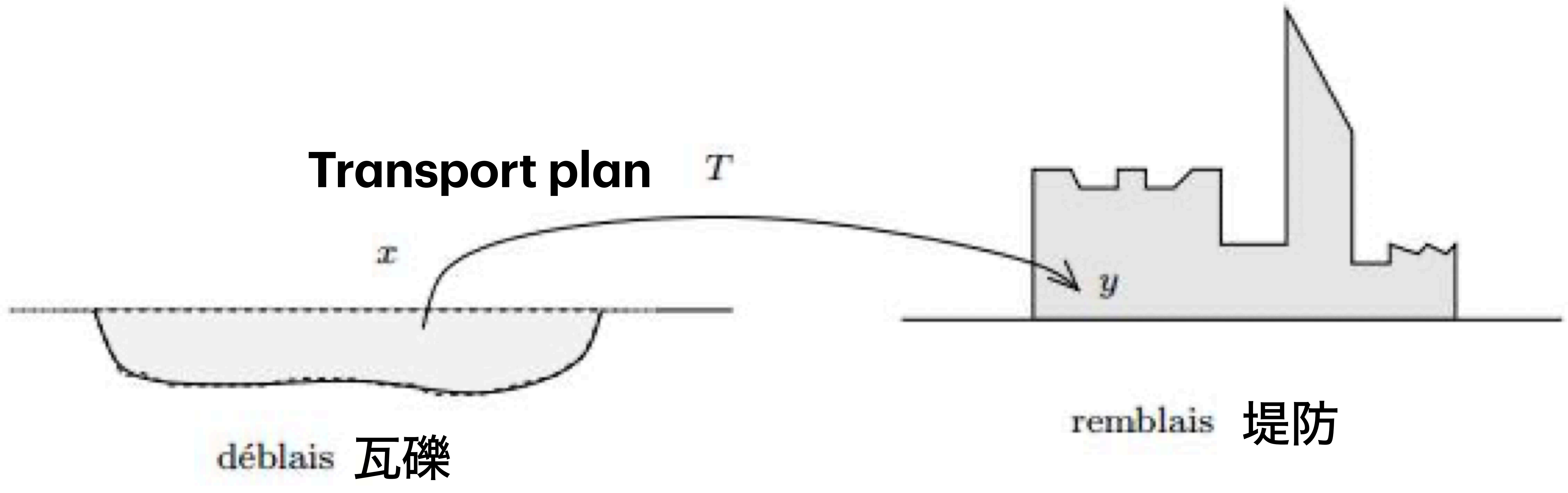
cf.
~500 pages

This is a standard textbook of the optimal transport theory written by Cédric Villani (Fields medalist in 2010).

It is somewhat challenging to introduce a lot of contents (~1000 pages) for physicists within 30mins. I will try!

What is the optimal transport?

Origin: Monge problem (1781)



Villani, C. (2009). *Optimal transport: old and new* (Vol. 338, p. 23). Berlin: springer.

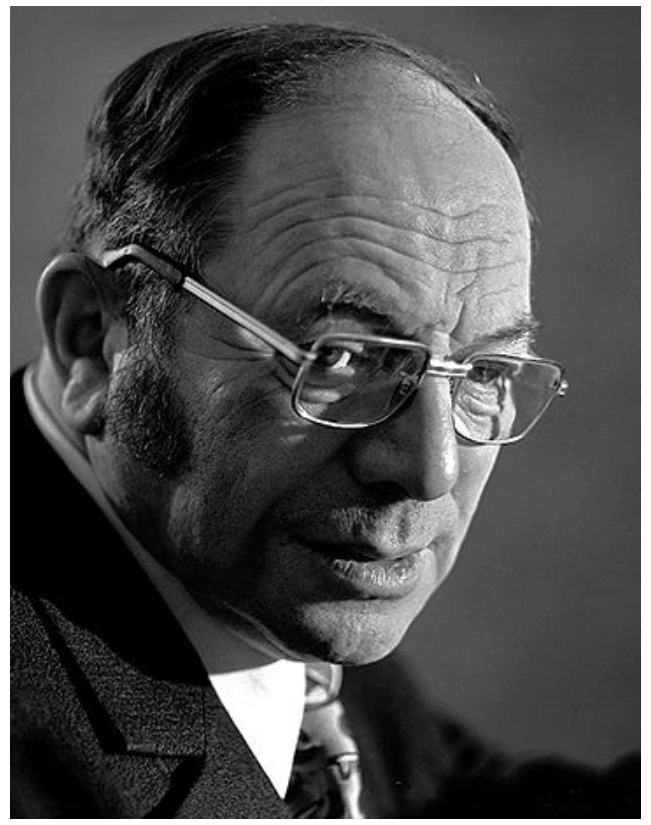
Gaspard Monge
1746-1818

We would like to move the sand from x (瓦礫) to y (堤防).

The transport cost depends on the distance from x to y.
What is the optimal transport plan y=T(x) to minimize the transport cost?

During the World War II

In 1939, L. Kantorovich became a professor at Military Engineering-Technical University in the Soviet Union, and was given the task of optimizing production in an industry.



Leonid Kantorovich
1912-1986

MATHEMATICAL METHODS OF ORGANIZING AND PLANNING PRODUCTION*†

L. V. KANTOROVICH

Introduction[1]

The immense tasks laid down in the plan for the third Five Year Plan period require that we achieve the highest possible production on the basis of the optimum utilization of the existing reserves of industry: materials, labor and equipment.

Optimum utilization of the existing reserves of industry; materials, labor and equipment (1939)

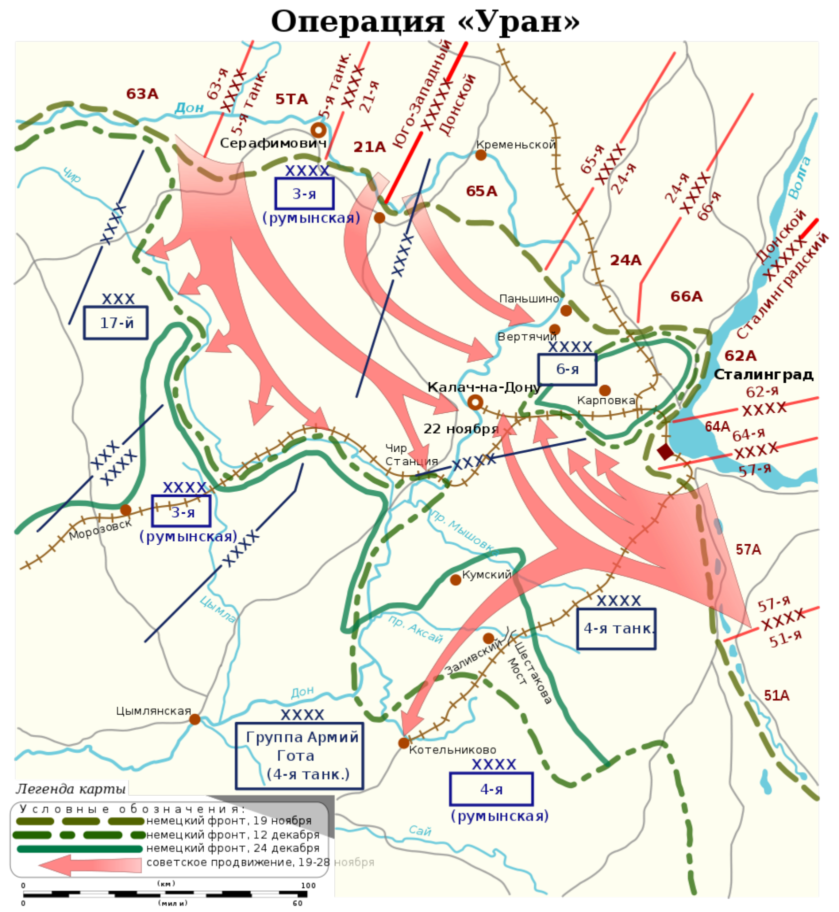
Nobel medals in 1975 (Economics)

ON THE TRANSLOCATION OF MASSES

L. V. Kantorovich*

The original paper was published in Dokl. Akad. Nauk SSSR, **37**, No. 7–8, 227–229 (1942).

Optimal translocation of masses (1942)



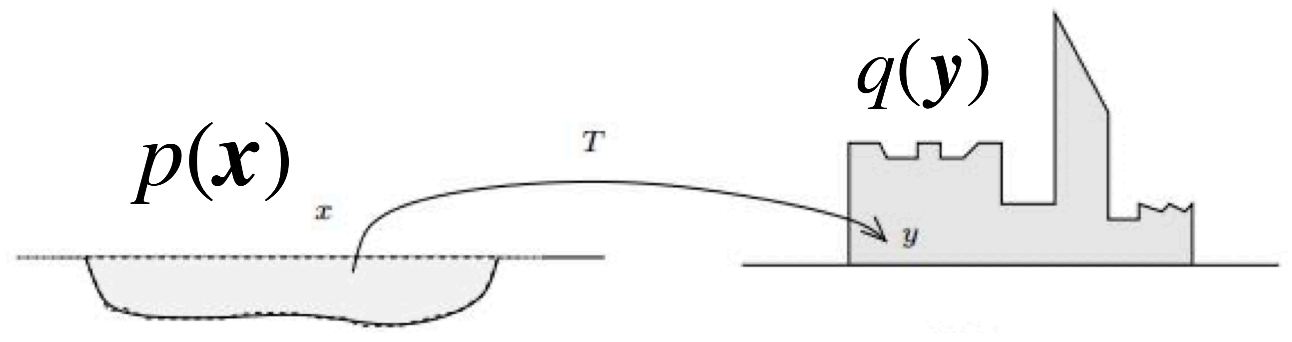
[Battle of Stalingrad in 1942]

(Image from wikipedia)

Monge-Kantorovich problem

Kantorovich's idea (1942)

$\boldsymbol{x} \in \mathbb{R}^d, \boldsymbol{y} \in \mathbb{R}^d, d \in \mathbb{N}$



Two probability distributions $p(\boldsymbol{x}), q(\boldsymbol{y})$

$$p(\boldsymbol{x}) \geq 0, q(\boldsymbol{y}) \geq 0 \quad \int d\boldsymbol{x} p(\boldsymbol{x}) = 1, \int d\boldsymbol{y} p(\boldsymbol{y}) = 1$$

Joint distribution $\Pi(\boldsymbol{x}, \boldsymbol{y})$ $\quad \Pi(\boldsymbol{x}, \boldsymbol{y}) \geq 0 \quad \int d\boldsymbol{x} \int d\boldsymbol{y} \Pi(\boldsymbol{x}) = 1$

$$\int d\boldsymbol{y} \Pi(\boldsymbol{x}, \boldsymbol{y}) = p(\boldsymbol{x}), \int d\boldsymbol{x} \Pi(\boldsymbol{x}, \boldsymbol{y}) = q(\boldsymbol{y})$$

Transport cost $c(\boldsymbol{x}, \boldsymbol{y}) \geq 0$

The work expended in transferring a unit mass from x to y (Kantorovich, 1942)

Monge-Kantorovich problem

$$C(p, q) = \inf_{\Pi} \int d\boldsymbol{x} d\boldsymbol{y} c(\boldsymbol{x}, \boldsymbol{y}) \Pi(\boldsymbol{x}, \boldsymbol{y})$$

L2 Wasserstein distance

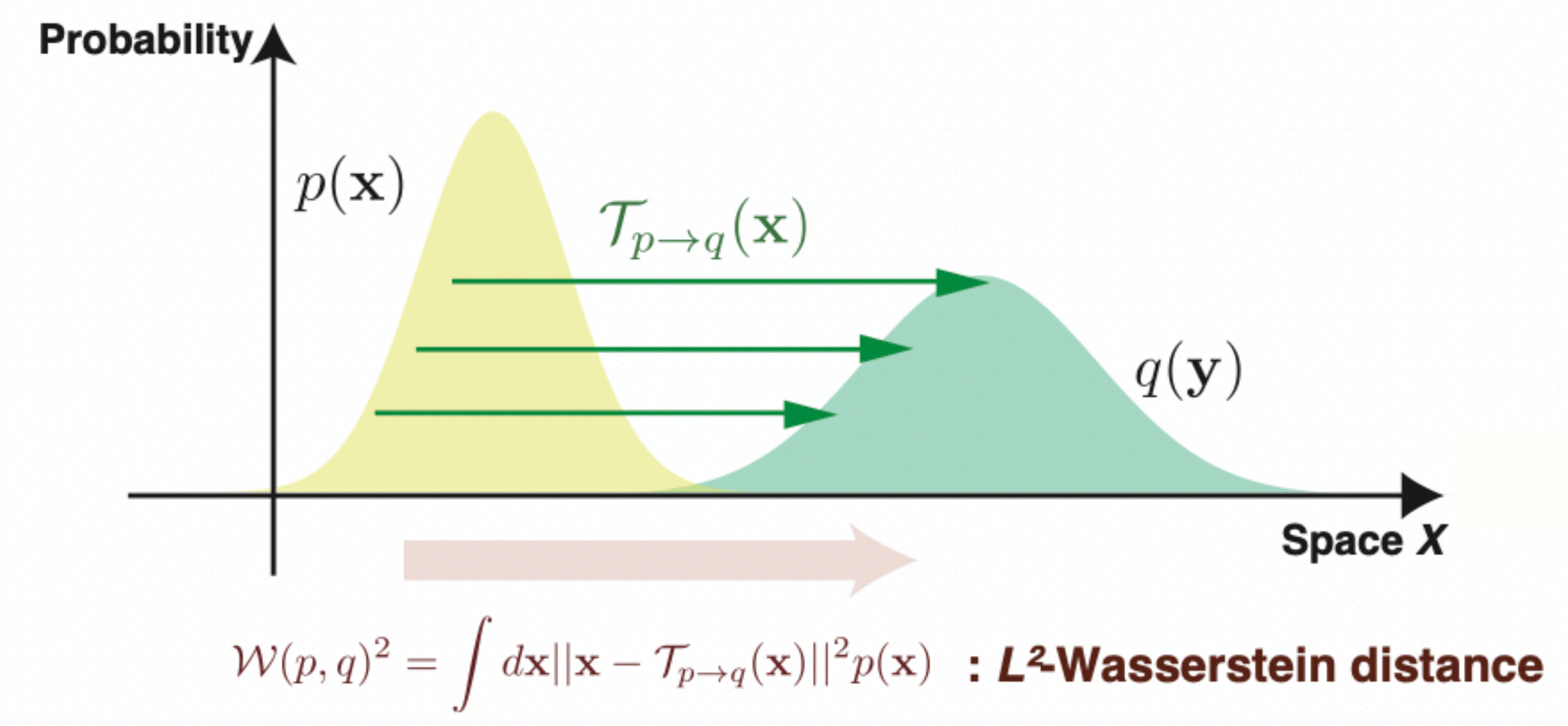
L2 Wasserstein distance $\mathscr{W}(p,q)$ (1969)

$$\sqrt{C(p,q)} = \mathscr{W}(p,q) \quad \text{such that} \quad c(\boldsymbol{x},\boldsymbol{y}) = ||\boldsymbol{x}-\boldsymbol{y}||^2$$

$$\mathscr{W}(p,q) = \sqrt{\inf_{\Pi} \int d\boldsymbol{x}d\boldsymbol{y}\, ||\boldsymbol{x}-\boldsymbol{y}||^2 \Pi(\boldsymbol{x},\boldsymbol{y})}$$

A solution
$$\Pi^*(\boldsymbol{x},\boldsymbol{y}) = \arg\min_{\Pi} \int d\boldsymbol{x}d\boldsymbol{y}\, ||\boldsymbol{x}-\boldsymbol{y}||^2 \Pi(\boldsymbol{x},\boldsymbol{y})$$

$$\Pi^*(\boldsymbol{x},\boldsymbol{y}) = \delta(\boldsymbol{y} - \mathscr{T}_{p\to q}(\boldsymbol{x}))p(\boldsymbol{x})$$



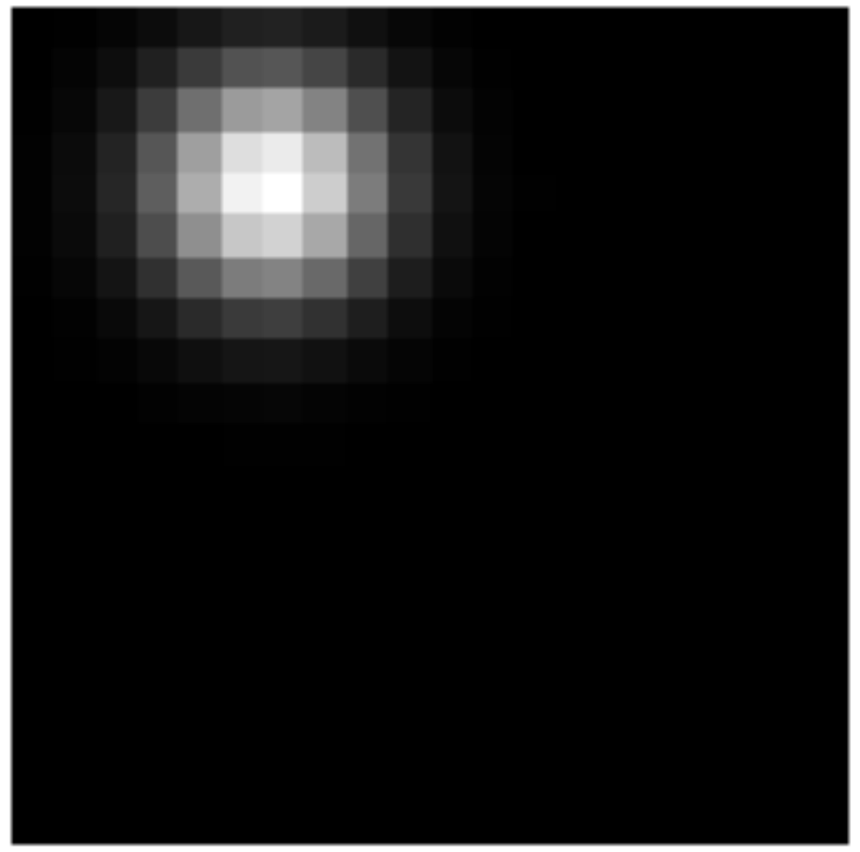
Distance between two distributions

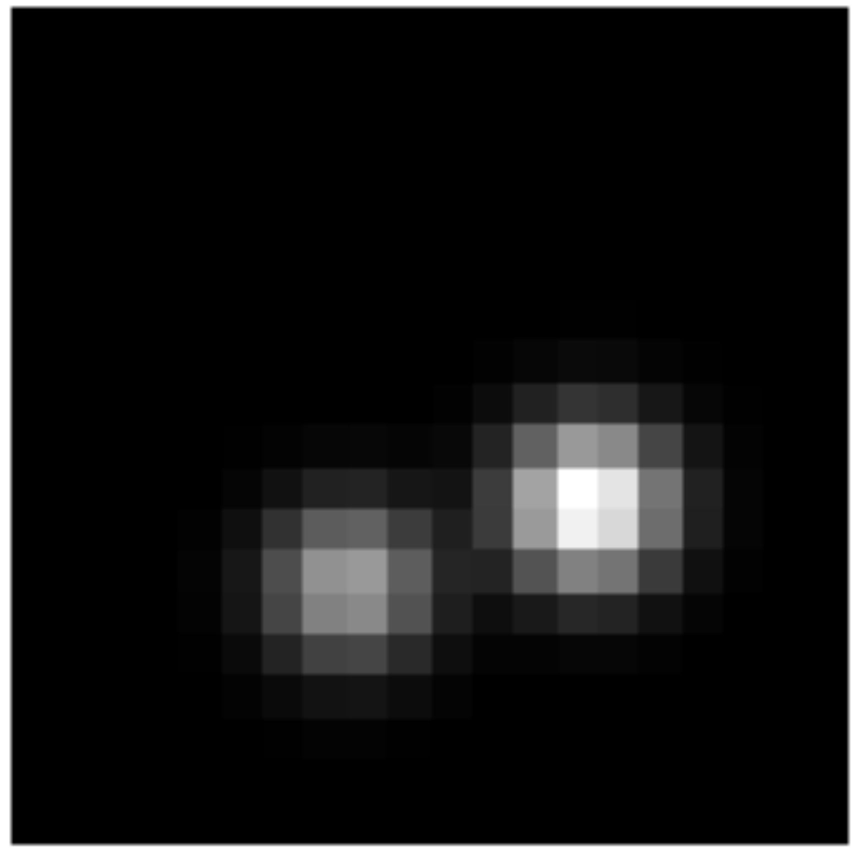
An existence of the optimal solution $\Pi^*(\boldsymbol{x},\boldsymbol{y})$ is mathematically proved if $\int d\boldsymbol{x}\,||\boldsymbol{x}||^2 p(\boldsymbol{x}) < \infty$, $\int d\boldsymbol{y}\,||\boldsymbol{y}||^2 q(\boldsymbol{y}) < \infty$. (Brenier 1987)

Why is the L2 Wasserstein distance important?

Two figures (as two probability distributions)

$p(x)$





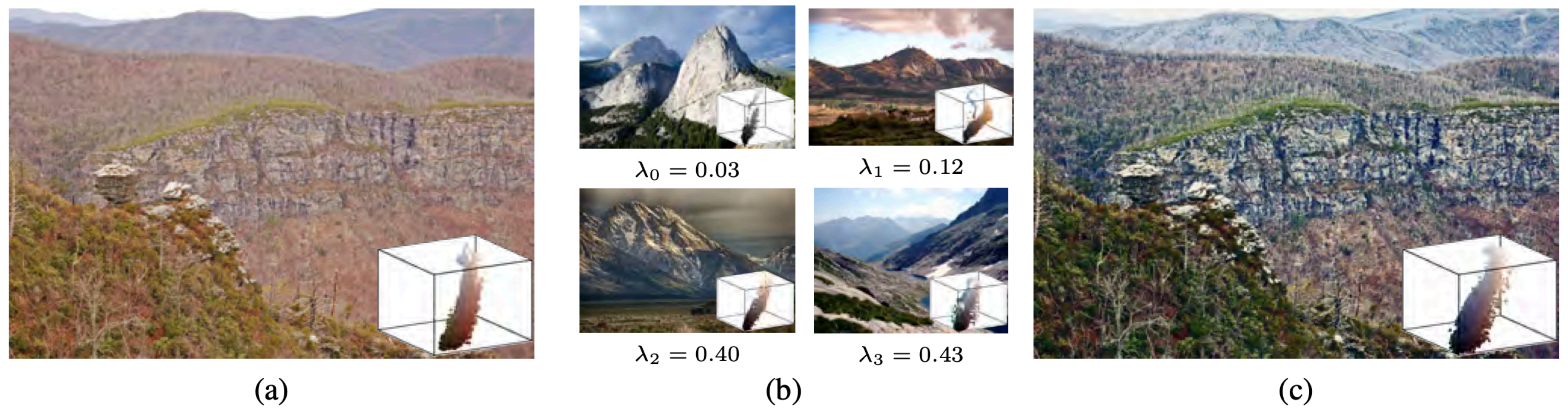
$q(y)$

$\mathscr{W}(p, q)$

https://www.numerical-tours.com/matlab/optimaltransp_2_benamou_brenier/

The L2 Wasserstein distance quantifies the difference between two figures.

$\Longrightarrow$ **A lot of applications**



Optimal transport plan to L2 Wasserstein distance

$$\mathscr{W}(p,q) = \sqrt{\int d\boldsymbol{x} \int d\boldsymbol{y}\, ||\boldsymbol{x} - \boldsymbol{y}||^2 \Pi^*(\boldsymbol{x},\boldsymbol{y})} = \sqrt{\int d\boldsymbol{x}\, ||\boldsymbol{x} - \mathscr{T}_{p\to q}(\boldsymbol{x})||^2 p(\boldsymbol{x})}$$

$$\Pi^*(\boldsymbol{x},\boldsymbol{y}) = \delta(\boldsymbol{y} - \mathscr{T}_{p\to q}(\boldsymbol{x}))p(\boldsymbol{x})$$

where the following Jacobian equation is satisfied.

$$p(\boldsymbol{x}) = q(\mathscr{T}_{p\to q}(\boldsymbol{x}))\,|\det(\nabla \mathscr{T}_{p\to q}(\boldsymbol{x}))|$$

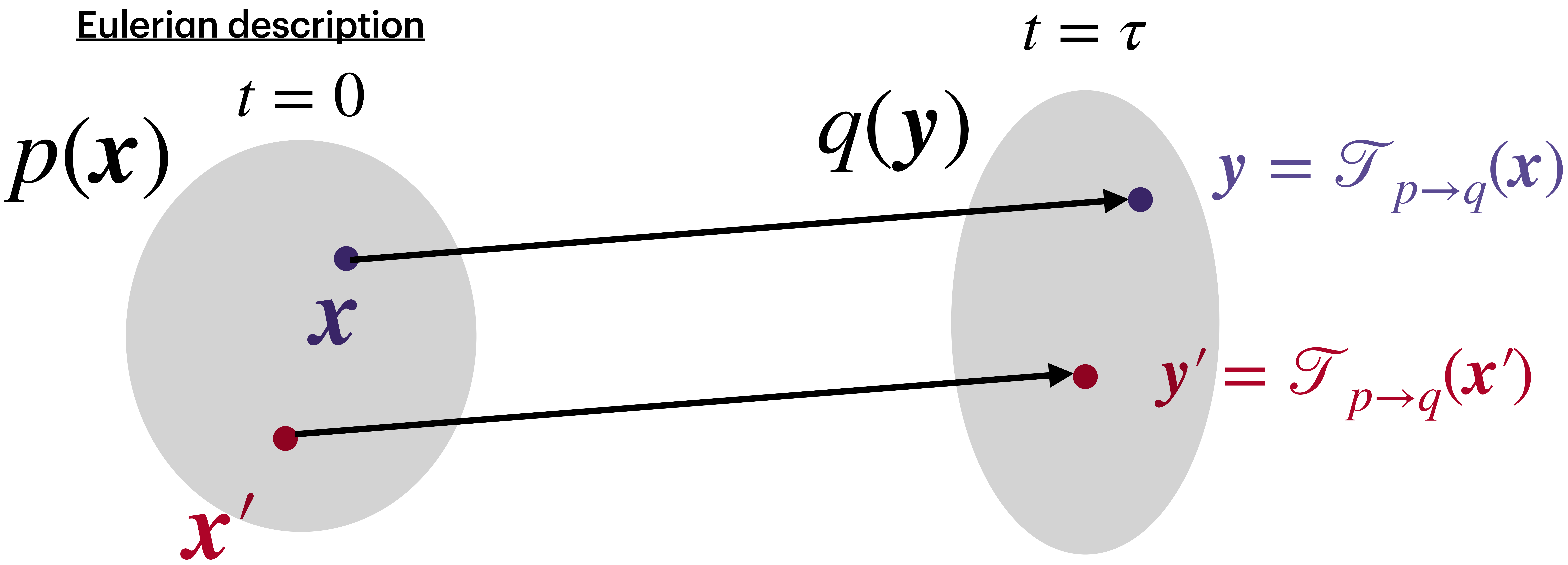
$\because$) **For any function** $f(\boldsymbol{x})$

$$\int d\boldsymbol{y} q(\boldsymbol{y}) f(\boldsymbol{y}) = \int d\boldsymbol{x} \int d\boldsymbol{y} f(\boldsymbol{y}) \Pi^*(\boldsymbol{x},\boldsymbol{y}) = \int d\boldsymbol{x} \int d\boldsymbol{y} f(\boldsymbol{y}) \delta(\boldsymbol{y} - \mathscr{T}_{p\to q}(\boldsymbol{x}))p(\boldsymbol{y}) = \int d\boldsymbol{x} f(\mathscr{T}_{p\to q}(\boldsymbol{x}))p(\mathscr{T}_{p\to q}(\boldsymbol{x}))$$

$$\boldsymbol{y} = \mathscr{T}_{p\to q}(\boldsymbol{x}), \quad d\boldsymbol{y} = |\det(\nabla \mathscr{T}_{p\to q}(\boldsymbol{x}))|\, d\boldsymbol{x}$$

How do we calculate it?

How do we calculate it? - Dynamical approach

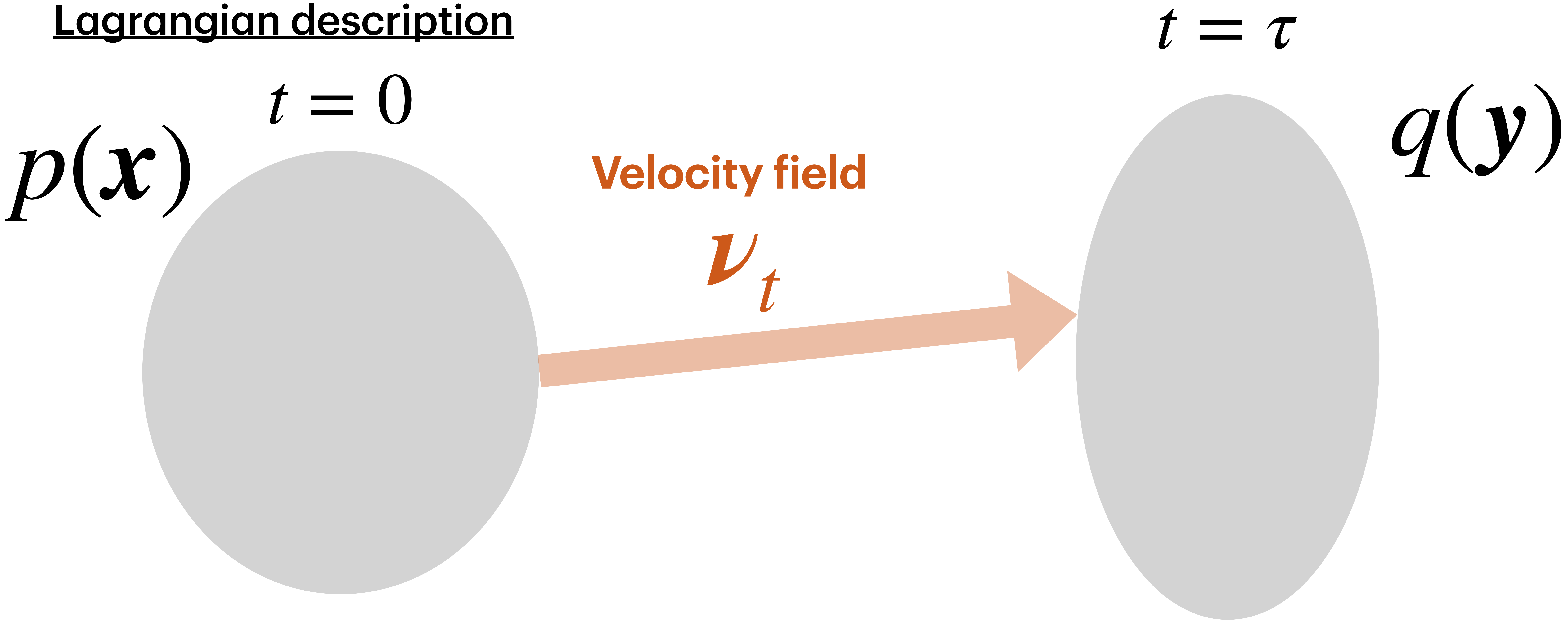


$$X(t,\boldsymbol{x}), X(0,\boldsymbol{x}) = \boldsymbol{x}, X(\tau,\boldsymbol{x}) = y = \mathcal{T}_{p\to q}(\boldsymbol{x})$$

We can consider dynamics of the optimal transport. [Material description]

How do we calculate it? - Dynamical approach

Lagrangian description



$$\partial_t P_t = -\nabla \cdot (\boldsymbol{\nu}_t P_t), \ \ P_0 = p, P_\tau = q$$

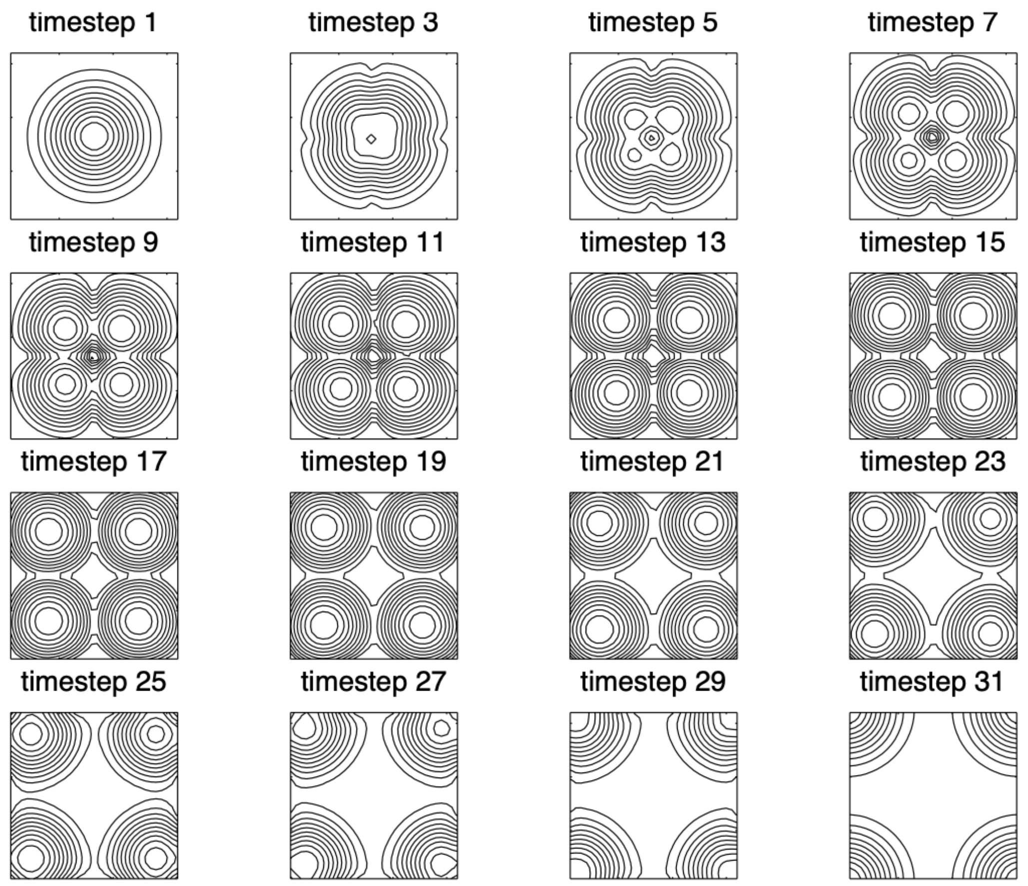
We also can consider “stochastic” dynamics of the optimal transport. [Spatial description]

Benamou-Brenier formula (2000)

$$\mathscr{W}(p,q) = \sqrt{\inf_{(\boldsymbol{\nu}_t, P_t)_{0\le t\le\tau}} \tau \int_0^\tau dt \int d\boldsymbol{x}\, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})}$$

such that $\partial_t P_t(\boldsymbol{x}) = -\nabla\cdot(\boldsymbol{\nu}_t(\boldsymbol{x})P_t(\boldsymbol{x})), \quad P_0(\boldsymbol{x}) = p(\boldsymbol{x}), P_\tau(\boldsymbol{x}) = q(\boldsymbol{x})$

This result gives the connection between the optimal transport theory and fluid dynamics.



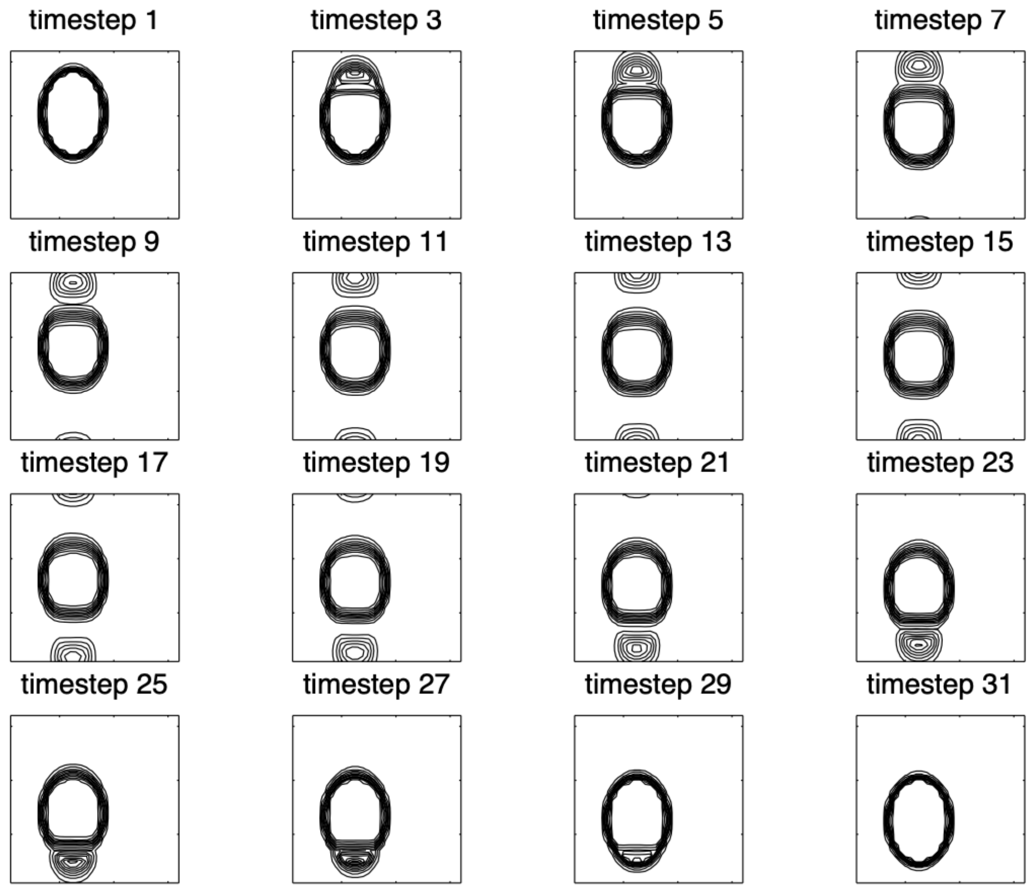


Fig. 3. Contours plots of the density at successive time steps

Benamou, Jean-David, and Yann Brenier. "A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem." *Numerische Mathematik* 84, 375-393 (2000).

Dynamics of the optimal velocity field $\boldsymbol{\nu}_t^*(\boldsymbol{x}) = \arg\min_{\boldsymbol{\nu}_t | \partial_t P_t = -\nabla\cdot(\boldsymbol{\nu}_t P_t)} \tau \int_0^\tau dt \int d\boldsymbol{x} \, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})$

Considering the following Lagrangian

$$\mathscr{L}[\{P_t\}, \{\boldsymbol{\nu}_t\}, \{\phi_t\}] = \int_0^\tau dt \int d\boldsymbol{x} \left[\frac{1}{2} ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) + \phi_t(\boldsymbol{x}) \left\{ \partial_t P_t(\boldsymbol{x}) + \nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x})) \right\} \right]$$

Variational calculus

$$\frac{\delta \mathscr{L}[\{P_t\}, \{\boldsymbol{\nu}_t\}, \{\phi_t\}]}{\delta\{P_t\}} = \frac{\delta \mathscr{L}[\{P_t\}, \{\boldsymbol{\nu}_t\}, \{\phi_t\}]}{\delta\{\nu_t\}} = \frac{\delta \mathscr{L}[\{P_t\}, \{\boldsymbol{\nu}_t\}, \{\phi_t\}]}{\delta\{\phi_t\}} = 0$$

Euler-Lagrange equation

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

$$\partial_t \phi_t(\boldsymbol{x}) + \frac{1}{2} ||\nabla \phi_t||^2 = 0$$

The Lagrange multiplier $\phi_t(x)$ can be regarded as the potential of the velocity field [Kantorovich potential].

(cf., pressure-less potential flow without vorticity in fluid mechanics)

Several faces of the L2 Wasserstein distance

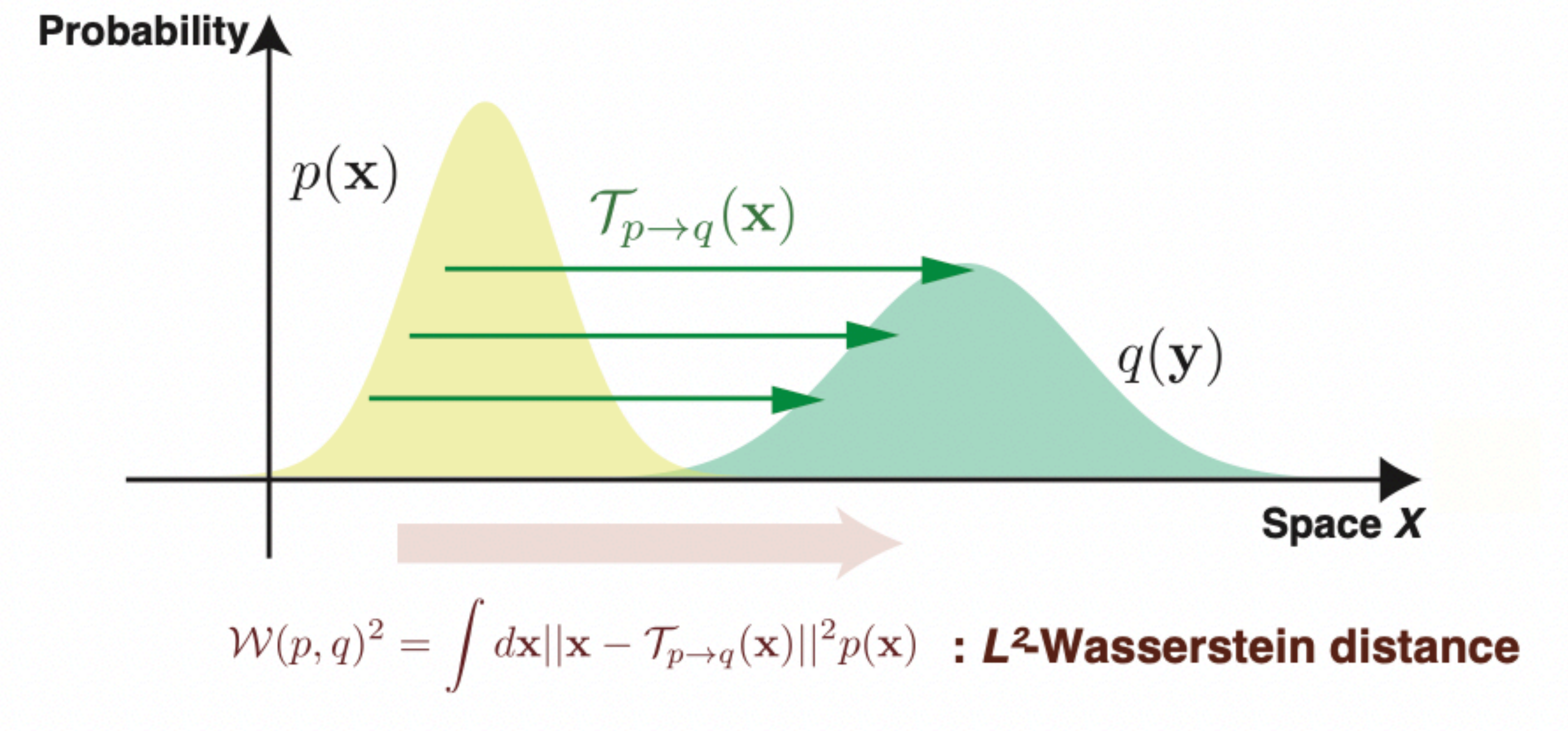
L2 Wasserstein distance

$$\mathscr{W}(p,q) = \sqrt{\inf_{\Pi} \int dxdy\,||\boldsymbol{x}-\boldsymbol{y}||^2 \Pi(\boldsymbol{x},\boldsymbol{y})}$$

$$= \sqrt{\int d\boldsymbol{x}\,||\boldsymbol{x} - \mathscr{T}_{p\to q}(\boldsymbol{x})||^2 p(\boldsymbol{x})}$$

$$= \sqrt{\inf_{\boldsymbol{\nu}_t | \partial_t P_t = -\nabla\cdot(\boldsymbol{\nu}_t P_t)} \tau \int_0^\tau dt \int d\boldsymbol{x}\,||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})}$$

$$= \sqrt{\tau \int_0^\tau dt \int d\boldsymbol{x}\,||\nabla\phi_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})}$$



$$\partial_t P_t(\boldsymbol{x}) = -\nabla\cdot([\nabla\phi_t(\boldsymbol{x})]P_t(\boldsymbol{x})),$$
$$P_0 = p, P_\tau = q$$
$$\partial_t\phi_t(\boldsymbol{x}) + \frac{1}{2}||\nabla\phi_t(\boldsymbol{x})||^2 = 0$$

Differential geometry

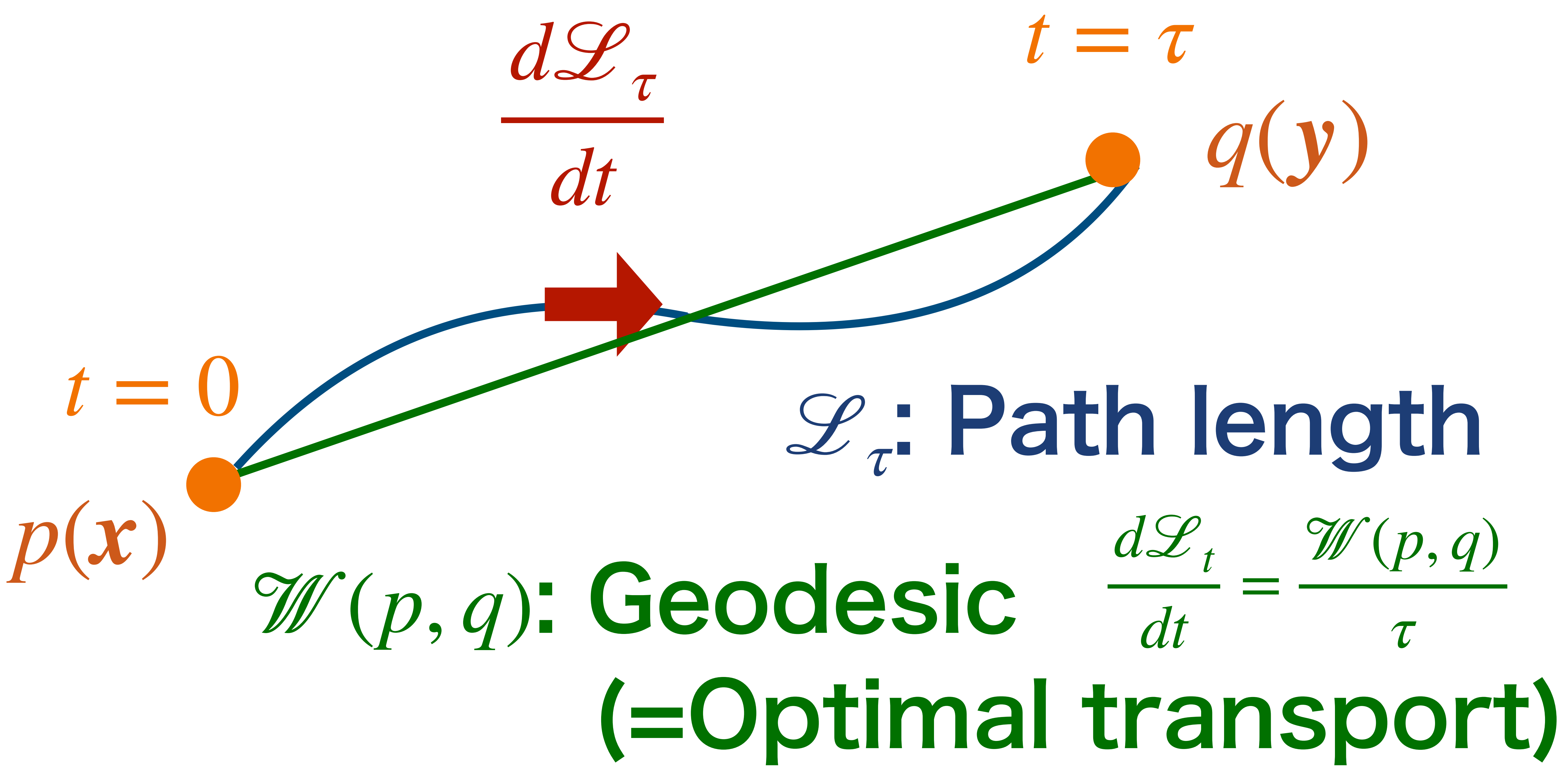
$$\mathscr{W}(p,q) = \sqrt{\tau \int_0^\tau dt \int d\boldsymbol{x} \, ||\nabla \phi_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})} \qquad \partial_t P_t(\boldsymbol{x}) = -\nabla \cdot ([\nabla \phi_t(\boldsymbol{x})] P_t(\boldsymbol{x})),$$

➡ $$\mathscr{W}^2(P_t, P_{t+\Delta t}) = (\Delta t)^2 \int d\boldsymbol{x} \, ||\nabla \phi_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) + O(\Delta t^3)$$

➡ $$\frac{d\mathscr{L}_\tau^2}{dt^2} = \lim_{\Delta t \to 0} \frac{\mathscr{W}^2(P_t, P_{t+\Delta t})}{(\Delta t)^2} = \int d\boldsymbol{x} \, ||\nabla \phi_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})$$

Triangle inequality:

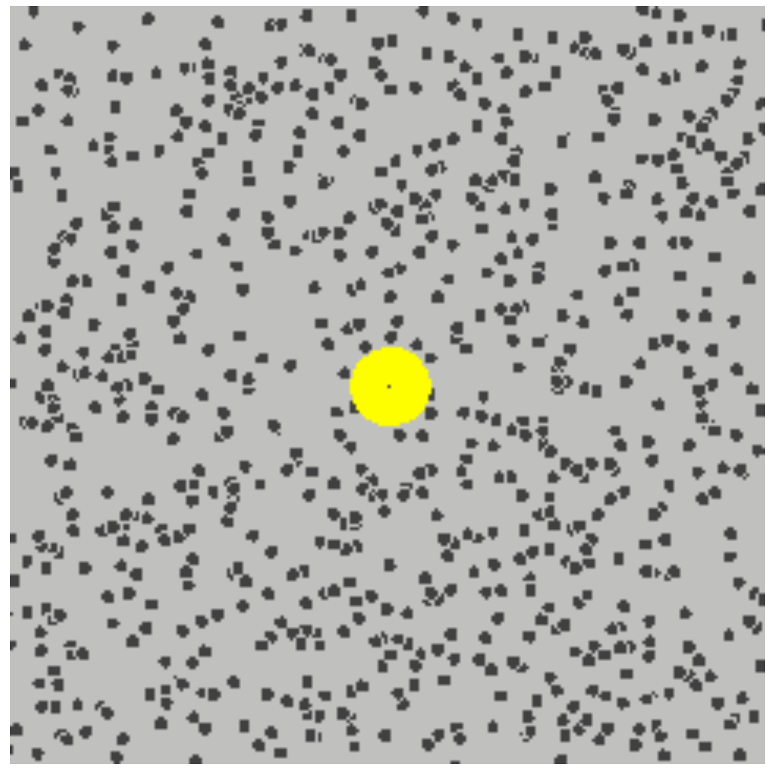
$$\mathscr{L}_\tau = \int_0^\tau \sqrt{\frac{d\mathscr{L}_t^2}{dt^2}} dt \geq \mathscr{W}(p,q)$$



- **Lecture on optimal transport theory (within 30 mins)**
- **Geometric theory of non-equilibirum thermodynamics**

Brownian motion

Random motion of the colloidal particle



(Image from wikipedia)

Relaxation to equilibrium

$$\boldsymbol{F}_t(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$$

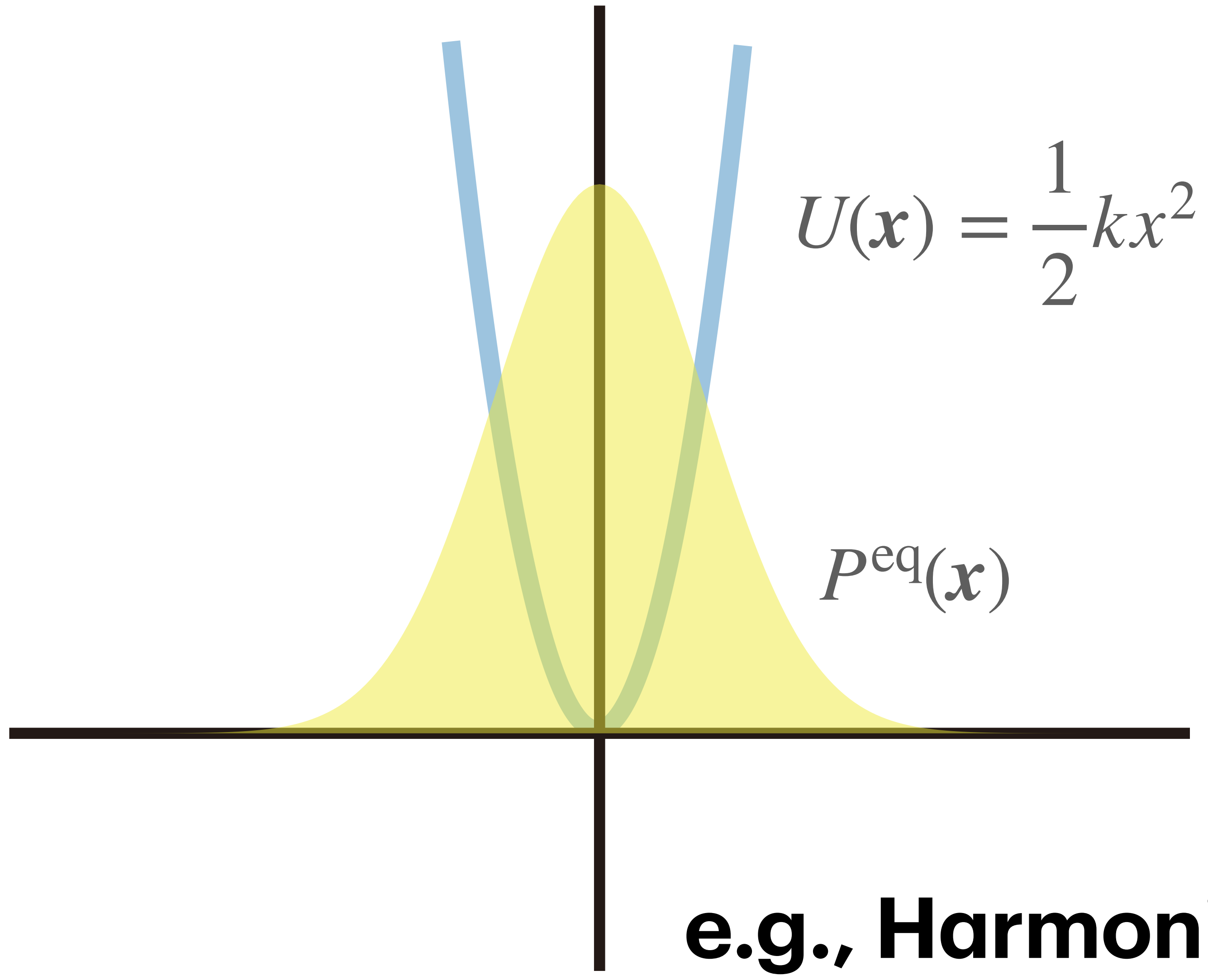
$$\lim_{t\to\infty} P_t(\boldsymbol{x}) = P^{\mathrm{eq}}(\boldsymbol{x}) = \frac{\exp(-\beta U(\boldsymbol{x}))}{\int d\boldsymbol{x} \exp(-\beta U(\boldsymbol{x}))}$$

Fokker-Planck equation [Spatial description]

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

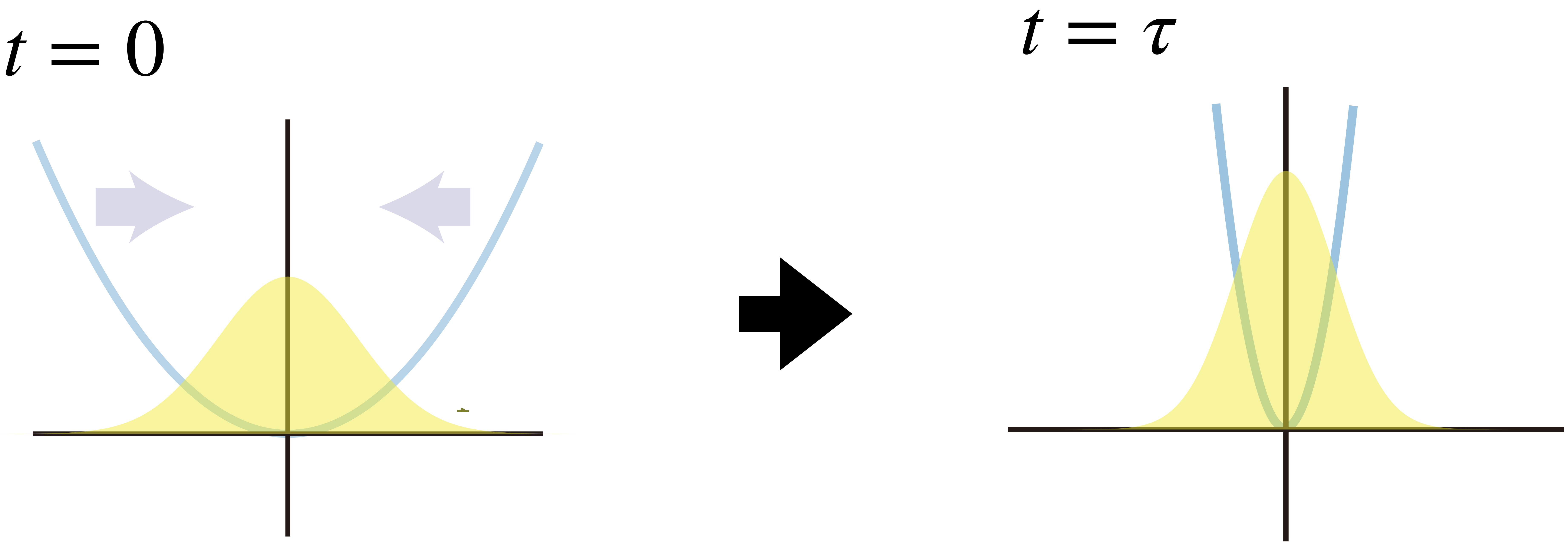
$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu(\boldsymbol{F}_t(\boldsymbol{x}) - \beta^{-1} \nabla \ln P_t(\boldsymbol{x}))$$

$\boldsymbol{F}_t(\boldsymbol{x})$**: Force,** β**: Inverse temperature,** μ **: Mobility**



e.g., Harmonic potential

Idea: Optimal tranport in Brownian motion



We control the probability distribution by using the change of the force $F_t(x)$.

Optimal transport problem → Minimizing a thermodynamic cost by the change of the force
= Minimum entropy production in finite time

Def. The entropy production

$$\Sigma_\tau = \frac{\beta}{\mu} \int_0^\tau dt \int d\boldsymbol{x} \, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x})$$

(≥ 0)

The second law of thermodynamics

A special case: the relaxation to equilibrium

Fokker-Planck equation [Spatial description]

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

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu(\boldsymbol{F}_t(\boldsymbol{x}) - \beta^{-1} \nabla \ln P_t(\boldsymbol{x}))$$

Relaxation to equilibrium

$$\boldsymbol{F}_t(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$$

$$\lim_{t \to \infty} P_t(\boldsymbol{x}) = P^{\mathrm{eq}}(\boldsymbol{x}) = \frac{\exp(-\beta U(\boldsymbol{x}))}{\int d\boldsymbol{x} \exp(-\beta U(\boldsymbol{x}))}$$

$$\Rightarrow \quad \boldsymbol{\nu}_t(\boldsymbol{x}) = \nabla \left[-\mu \beta^{-1} \ln \frac{P_t(\boldsymbol{x})}{P^{\mathrm{eq}}(\boldsymbol{x})} \right] = \nabla \phi_t(\boldsymbol{x})$$

Optimal transport (in an infinitesimal time interval)

Wasserstein geometry

$$\frac{ds^2}{dt^2} = \lim_{\Delta t \to 0} \frac{\mathscr{W}^2(P_t, P_{t+\Delta t})}{(\Delta t)^2} = \int d\boldsymbol{x} \, || \nabla \phi_t(\boldsymbol{x}) ||^2 P_t(\boldsymbol{x})$$

$$= -\mu \beta^{-1} \int d\boldsymbol{x} \ln \frac{P_t(\boldsymbol{x})}{P^{\mathrm{eq}}(\boldsymbol{x})} \nabla \cdot ([\nabla \phi_t(\boldsymbol{x})] P_t(\boldsymbol{x})) = -(\mu \beta^{-1}) \frac{d}{dt} \int d\boldsymbol{x} P_t(\boldsymbol{x}) \ln \frac{P_t(\boldsymbol{x})}{P^{\mathrm{eq}}(\boldsymbol{x})}$$

$$:= D_{\mathrm{KL}}(P_t || P^{\mathrm{eq}})$$

KL divergence between $P_t(\boldsymbol{x})$ and $P^{\mathrm{eq}}(\boldsymbol{x})$

The Wasserstein geometry and the entropy production rate

M. Nakazato, and SI. *Physical Review Research* 3, 043093 (2021).

For the case of the relaxation to equilibrium $F_t(\boldsymbol{x}) = -\nabla U(\boldsymbol{x})$

The entropy production rate

$$\sigma_t := \left.\frac{d\Sigma_\tau}{d\tau}\right|_{\tau=t} = -\frac{d}{dt} D_{\mathrm{KL}}(P_t || P^{\mathrm{eq}}) = \frac{\beta}{\mu} \lim_{\Delta t \to 0} \frac{\mathscr{W}^2(P_t, P_{t+\Delta t})}{(\Delta t)^2} = \frac{\beta}{\mu}\frac{d\mathscr{L}_\tau^2}{dt^2}$$

is a geometric quantity.

The entropy production

$$\Sigma_\tau = \frac{\beta}{\mu}\int_0^\tau dt \frac{d\mathscr{L}_\tau^2}{dt^2}$$

In general $F_t(\boldsymbol{x}) \neq -\nabla U(\boldsymbol{x})$ It is an inequality.

$$\Sigma_t \geq \frac{\beta}{\mu}\int_0^\tau dt \frac{d\mathscr{L}_\tau^2}{dt^2}$$

$$\because) \quad \sigma_t = \frac{\beta}{\mu}\int d\boldsymbol{x}\, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) \geq \frac{\beta}{\mu}\inf_{\boldsymbol{\nu}_t | \partial_t P_t = -\nabla\cdot(\boldsymbol{\nu}_t P_t)} \int d\boldsymbol{x}\, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) = \frac{\beta}{\mu}\lim_{\Delta t \to 0}\frac{\mathscr{W}^2(P_t, P_{t+\Delta t})}{(\Delta t)^2} = \frac{\beta}{\mu}\frac{d\mathscr{L}_\tau^2}{dt^2}$$

The trade-off relation between time and dissipation

Thermodynamic speed limit [Aurell et al. 2011] (= Benamou-Brenier formula)

$$\Sigma_\tau = \frac{\beta}{\mu}\int_0^\tau dt \int dx\, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) \geq \frac{\beta}{\mu\tau}\inf_{\boldsymbol{\nu}_t} \tau \int_0^\tau dt \int dx\, ||\boldsymbol{\nu}_t(\boldsymbol{x})||^2 P_t(\boldsymbol{x}) = \frac{\beta \mathscr{W}^2(P_0, P_\tau)}{\mu\tau} (\geq 0)$$

This is a lower bound on the entropy production for the finite time transition, which is tighter than the second law.

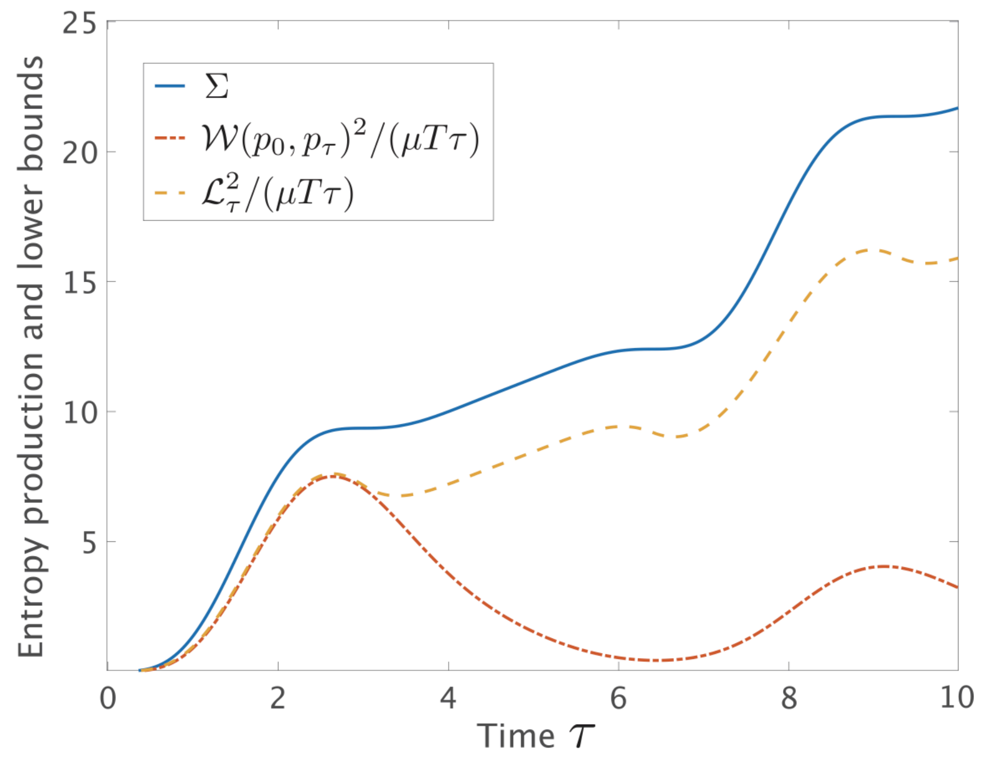
Aurell, E., Mejía-Monasterio, C., & Muratore-Ginanneschi, P. Optimal protocols and optimal transport in stochastic thermodynamics. *Physical review letters*, *106*(25), 250601 (2011).

Our tighter bound

$$\Sigma_\tau \geq \frac{\beta(\mathscr{L}_\tau)^2}{\mu\tau}\left(\geq \frac{\beta \mathscr{W}^2(P_0, P_\tau)}{\mu\tau}\right)$$

$$\because)\ \Sigma_\tau = \int_0^\tau dt \sigma_t \geq \frac{\beta}{\mu}\int_0^\tau dt \frac{d\mathscr{L}_t^2}{dt^2} \geq \frac{\beta}{\mu}\frac{\left(\int_0^\tau \frac{d\mathscr{L}_t}{dt}\right)^2}{\int_0^\tau dt} = \frac{\beta(\mathscr{L}_\tau)^2}{\mu\tau} \geq \frac{\beta \mathscr{W}^2(P_0, P_\tau)}{\mu\tau}$$

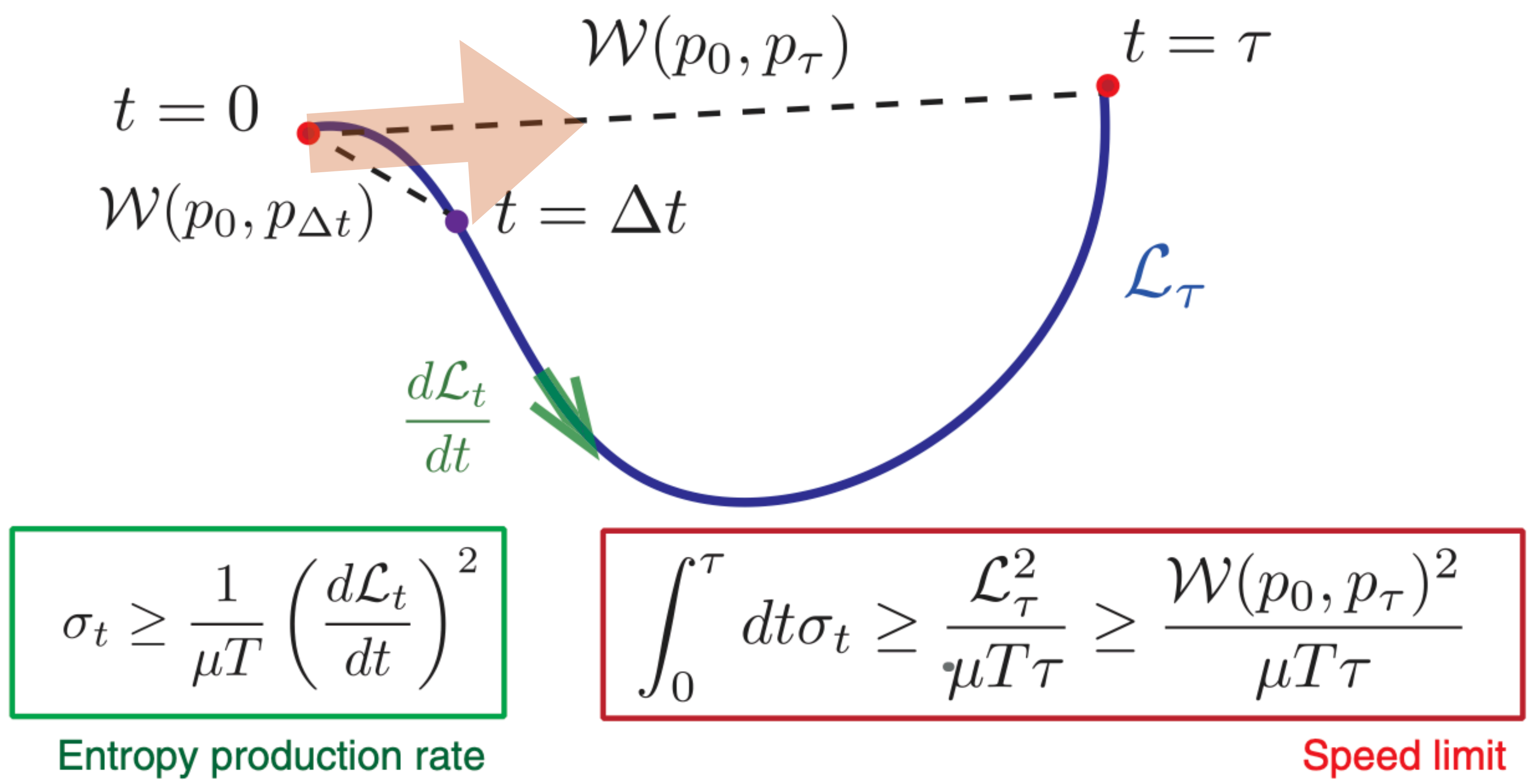
↑ Cauchy-Schwarz inequality



M. Nakazato, and SI. *Physical Review Research* 3, 043093 (2021).

The geometric optimal protocol to minimize entropy production

Optimal protocol (Geodesic, Constant speed)



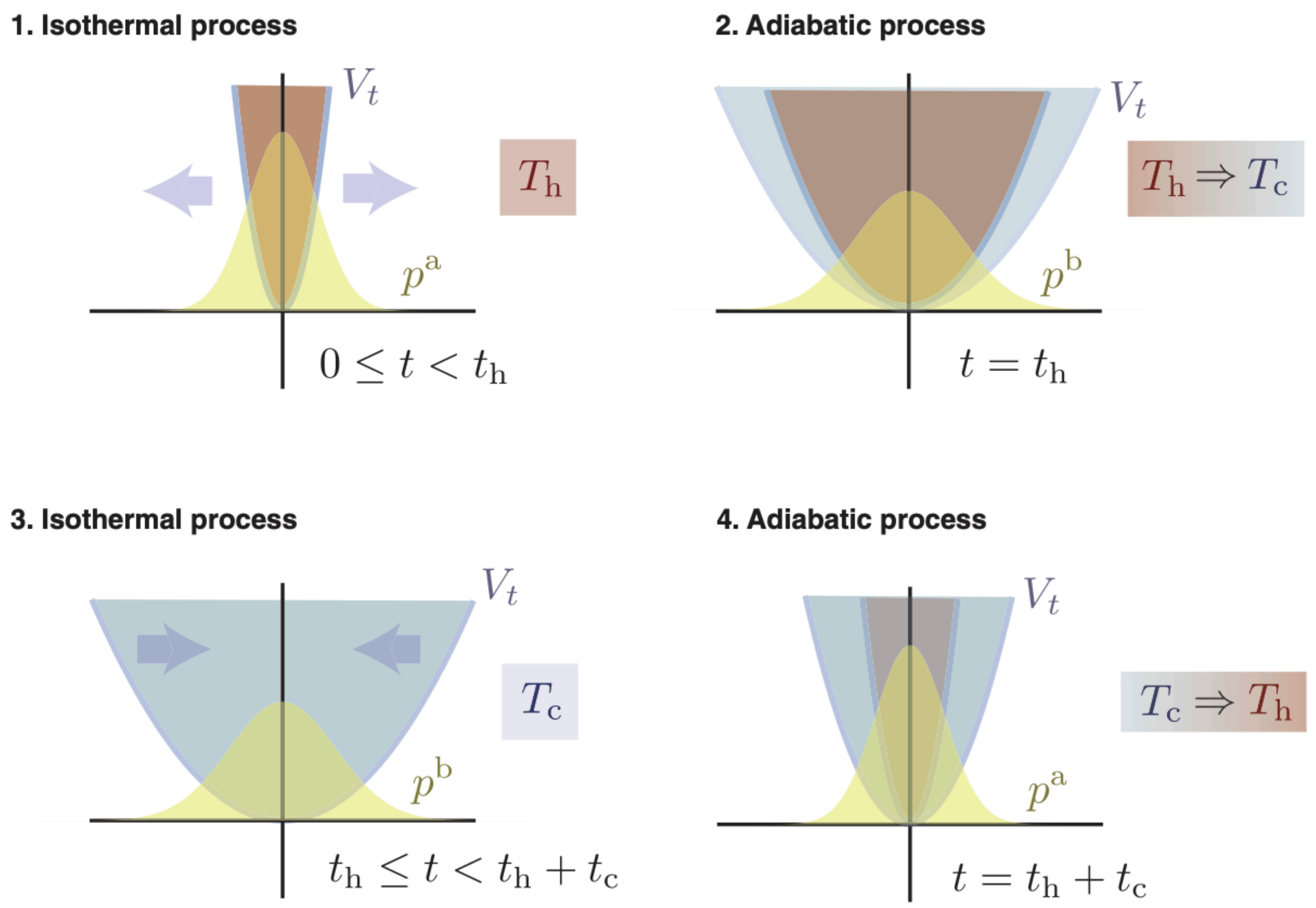
Optimal protocol

$$\nu_t(\boldsymbol{x}) = \nabla \phi_t(\boldsymbol{x})$$

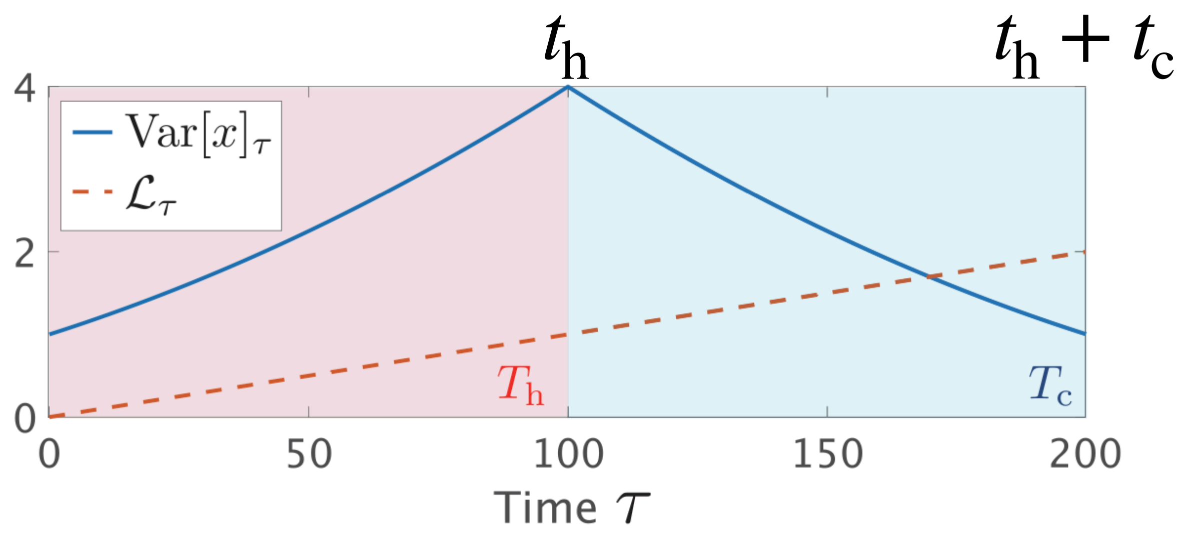
$$\frac{d\mathscr{L}_t}{dt} = \frac{\mathscr{W}(P_0, P_\tau)}{\tau}$$

e.g., Brownian heat engine

Maximum efficiency in finite time $\tau = t_\mathrm{h} + t_\mathrm{c}$ can be achieved when $\frac{d\mathscr{L}_t}{dt} = \mathrm{const.}$.



$$\eta_{\max} = \frac{T_\mathrm{h} - T_\mathrm{c} - \frac{\mathscr{W}(p^a, p^b)}{\mu(t_\mathrm{h}^{-1} + t_\mathrm{c}^{-1})^{-1}\Delta S}}{T_\mathrm{h} - \frac{\mathscr{W}(p^a, p^b)}{\mu t_\mathrm{h}\Delta S}} \leq \frac{T_\mathrm{h} - T_\mathrm{c}}{T_\mathrm{h}}$$



$$\Delta S = \int d\boldsymbol{x} p^a(\boldsymbol{x}) \ln p^a(\boldsymbol{x}) - \int d\boldsymbol{x} p^b(\boldsymbol{x}) \ln p^b(\boldsymbol{x})$$

M. Nakazato, and SI. *Physical Review Research* 3, 043093 (2021).

The geometric decomposition

A. Dechant, S-I Sasa, and SI. *Physical Review Research* 4, L012034 (2022). A. Dechant, S-I Sasa, and SI. *arXiv:2202.04331* (2022).

$$\sigma_t \geq \frac{\beta}{\mu}\frac{d\mathscr{L}_\tau^2}{dt^2} \quad \Rightarrow \quad \sigma_t = \underbrace{\frac{\beta}{\mu}\frac{d\mathscr{L}_\tau^2}{dt^2}}_{:= \sigma_t^{\mathrm{ex}} \geq 0} + \underbrace{\left(\sigma_t - \frac{\beta}{\mu}\frac{d\mathscr{L}_\tau^2}{dt^2}\right)}_{:= \sigma_t^{\mathrm{hk}} \geq 0}$$

Two nonnegative terms

Excess **Housekeeping**

Fokker-Planck equation

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

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

e.g., The Helmholtz decomposition for three dimension ($\boldsymbol{x} \in \mathbb{R}^3$)

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \nabla \phi_t(\boldsymbol{x}) + \frac{\nabla \times \boldsymbol{A}_t(\boldsymbol{x})}{P_t(\boldsymbol{x})}$$

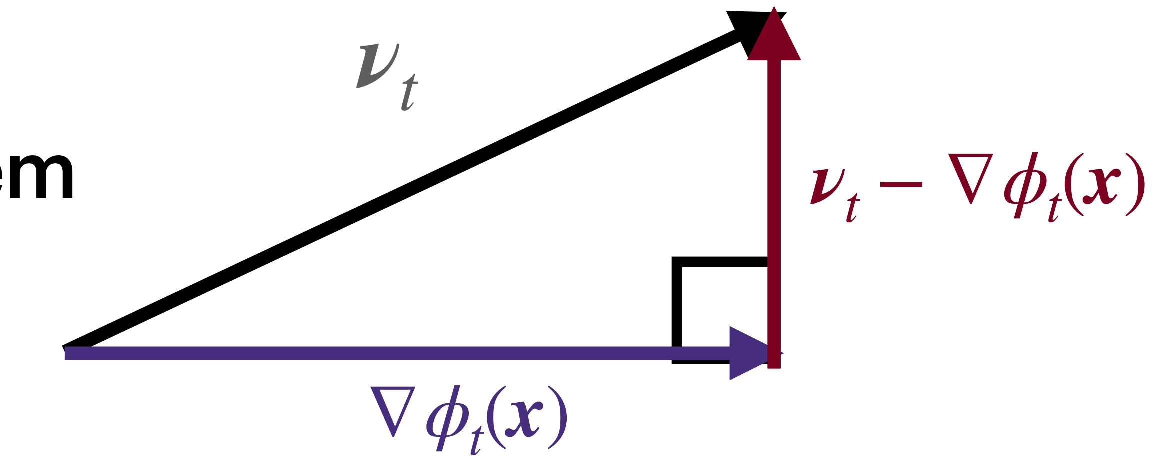
Orthogonality (e.g., Scalar potential and vector potential in the Helmholtz decomposition)

$$\langle \nabla \phi_t, \boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla \phi_t \rangle_{P_t} = 0$$

Inner product $\langle \boldsymbol{a}, \boldsymbol{b} \rangle_{P_t} := \frac{\beta}{\mu} \int d\boldsymbol{x}\, \boldsymbol{a}(\boldsymbol{x}) \cdot \boldsymbol{b}(\boldsymbol{x}) P_t(\boldsymbol{x})$

$$\sigma_t = \langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle_{P_t} = \underbrace{\langle \nabla \phi_t, \nabla \phi_t \rangle_{P_t}}_{:= \sigma_t^{\mathrm{ex}} \geq 0} + \underbrace{\langle \boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla \phi_t, \boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla \phi_t \rangle_{P_t}}_{:= \sigma_t^{\mathrm{hk}} \geq 0} = \sigma_t^{\mathrm{ex}} + \sigma_t^{\mathrm{hk}}$$

Pythagorean theorem



Thermodynamic uncertainty relations

A. Dechant, S-I Sasa, and SI. *Physical Review Research* 4, L012034 (2022). A. Dechant, S-I Sasa, and SI. *arXiv:2202.04331* (2022).

For any observable $R(\boldsymbol{x})$

$$\langle \nabla \phi_t, \nabla R \rangle_{P_t} = \int d\boldsymbol{x} \nabla \phi_t \cdot \nabla R(\boldsymbol{x}) P_t(\boldsymbol{x}) = \int d\boldsymbol{x} R(\boldsymbol{x}) \partial_t P_t(\boldsymbol{x}) = \frac{d}{dt} \mathbb{E}_{P_t}[R] \qquad \mathbb{E}_{P_t}[R] = \int d\boldsymbol{x} R(\boldsymbol{x}) P_t(\boldsymbol{x})$$

Thermodynamic uncertainty relation

$$\sigma_t \geq \sigma_t^{\mathrm{ex}} \geq \frac{\left(\frac{d}{dt} \mathbb{E}_{P_t}[R] \right)^2}{\langle \nabla R, \nabla R \rangle_{P_t}}$$

$\because$) $$\langle \boldsymbol{\nu}_t, \boldsymbol{\nu}_t \rangle_{P_t} \geq \langle \nabla \phi_t, \nabla \phi_t \rangle_{P_t} \geq \frac{(\langle \nabla \phi_t, \nabla R \rangle_{P_t})^2}{\langle \nabla R, \nabla R \rangle_{P_t}}$$

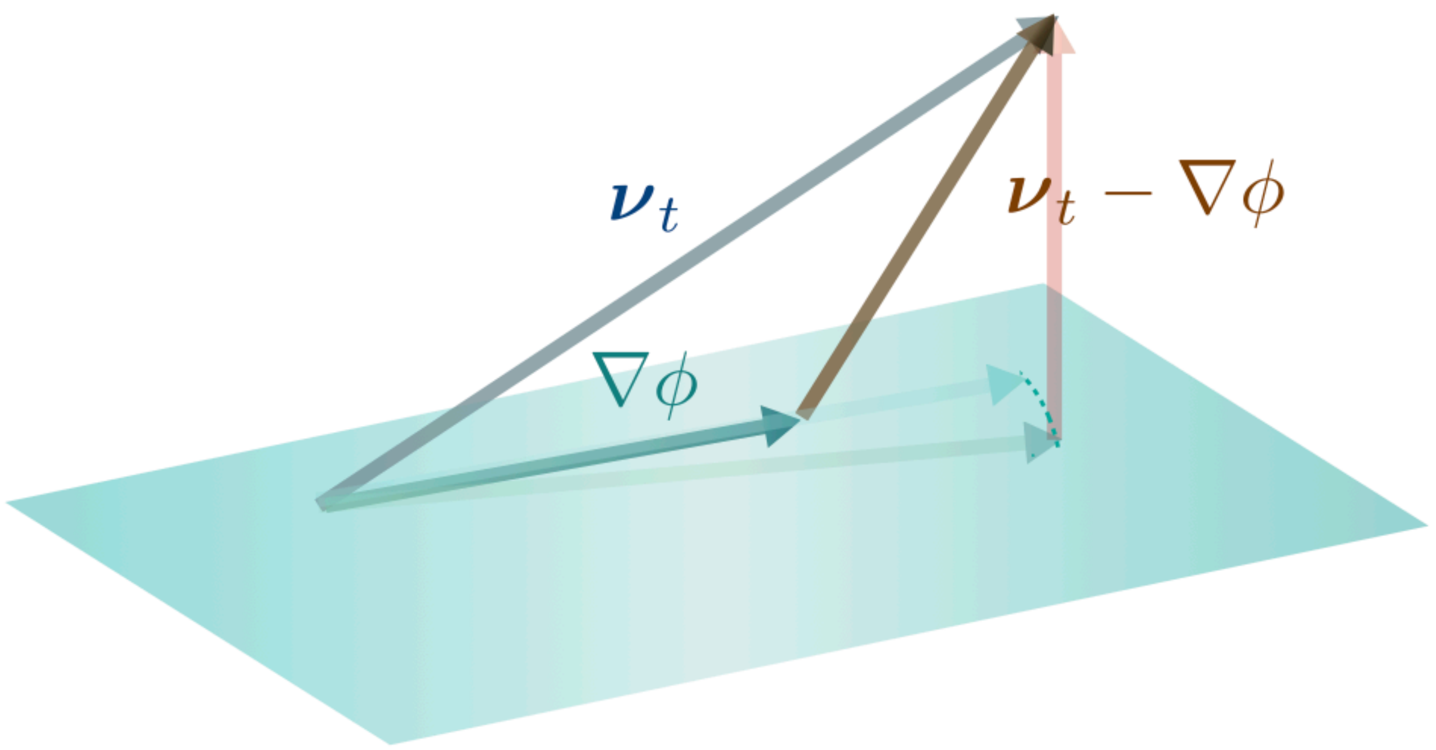
↑ Cauchy-Schwarz inequality

A trade-off relation among fluctuation $\langle \nabla R, \nabla R \rangle_{P_t}$, speed $\left| \frac{d}{dt} \mathbb{E}_{P_t}[R] \right|$ and entropy production rate σ_t.

Variational formulas

A. Dechant, S-I Sasa, and SI. *Physical Review Research* 4, L012034 (2022). A. Dechant, S-I Sasa, and SI. *arXiv:2202.04331* (2022).

$$V^{(1)} = \{ \boldsymbol{u} \mid \boldsymbol{u} = \nabla \phi \} \qquad V^{(2)} = \{ \boldsymbol{u} \mid \langle \boldsymbol{\nu}, \boldsymbol{u} \rangle_{P_t} = 0, \boldsymbol{\nu} \in V^{(1)} \}$$



$$\sigma_t^{\mathrm{ex}} = \sup_{\boldsymbol{u} \in V^{(1)}} \left(\frac{\langle \boldsymbol{u}, \boldsymbol{\nu}_t \rangle_{P_t}^2}{\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{P_t}} \right) = \inf_{\boldsymbol{u} \in V^{(2)}} \langle \boldsymbol{\nu}_t - \boldsymbol{u}, \boldsymbol{\nu}_t - \boldsymbol{u} \rangle_{P_t}$$

$$= \sup_{\phi_t} \left(\frac{\langle \nabla \phi_t, \boldsymbol{\nu}_t \rangle_{P_t}^2}{\langle \nabla \phi_t, \nabla \phi_t \rangle_{P_t}} \right)$$

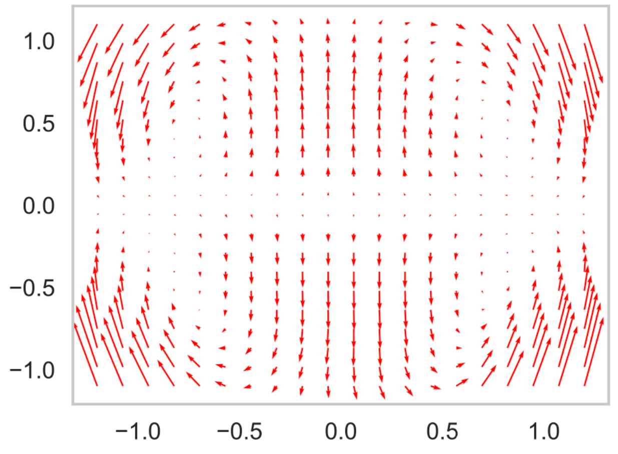
The upper bound of the thermodynamic uncertainty relation

$$\sigma_t^{\mathrm{hk}} = \sup_{\boldsymbol{u} \in V^{(2)}} \left(\frac{\langle \boldsymbol{u}, \boldsymbol{\nu}_t \rangle_{P_t}^2}{\langle \boldsymbol{u}, \boldsymbol{u} \rangle_{P_t}} \right) = \inf_{\boldsymbol{u} \in V^{(1)}} \langle \boldsymbol{\nu}_t - \boldsymbol{u}, \boldsymbol{\nu}_t - \boldsymbol{u} \rangle_{P_t} = \inf_{\phi_t} \langle \boldsymbol{\nu}_t - \nabla \phi_t, \boldsymbol{\nu}_t - \nabla \phi_t \rangle_{P_t}$$

These formulas might be useful to obtain these quantities from the experimental data by the machine learning.

e.g.,) S. Otsubo, SI., A. Dechant and T. Sagawa, *Physical Review E, 101*(6), 062106 (2020).

Estimation of the entropy production based on the upper bound of the thermodynamic uncertainty relation.



Estimation of the velocity field $\boldsymbol{\nu}_t$

A generalization for the discrete state

K. Yoshimura, A. Kolchinsky, A. Dechant, and SI. *arXiv:2205.15227* (2022).

A generalization for the master equation (or the deterministic rate equation for chemical reaction networks)

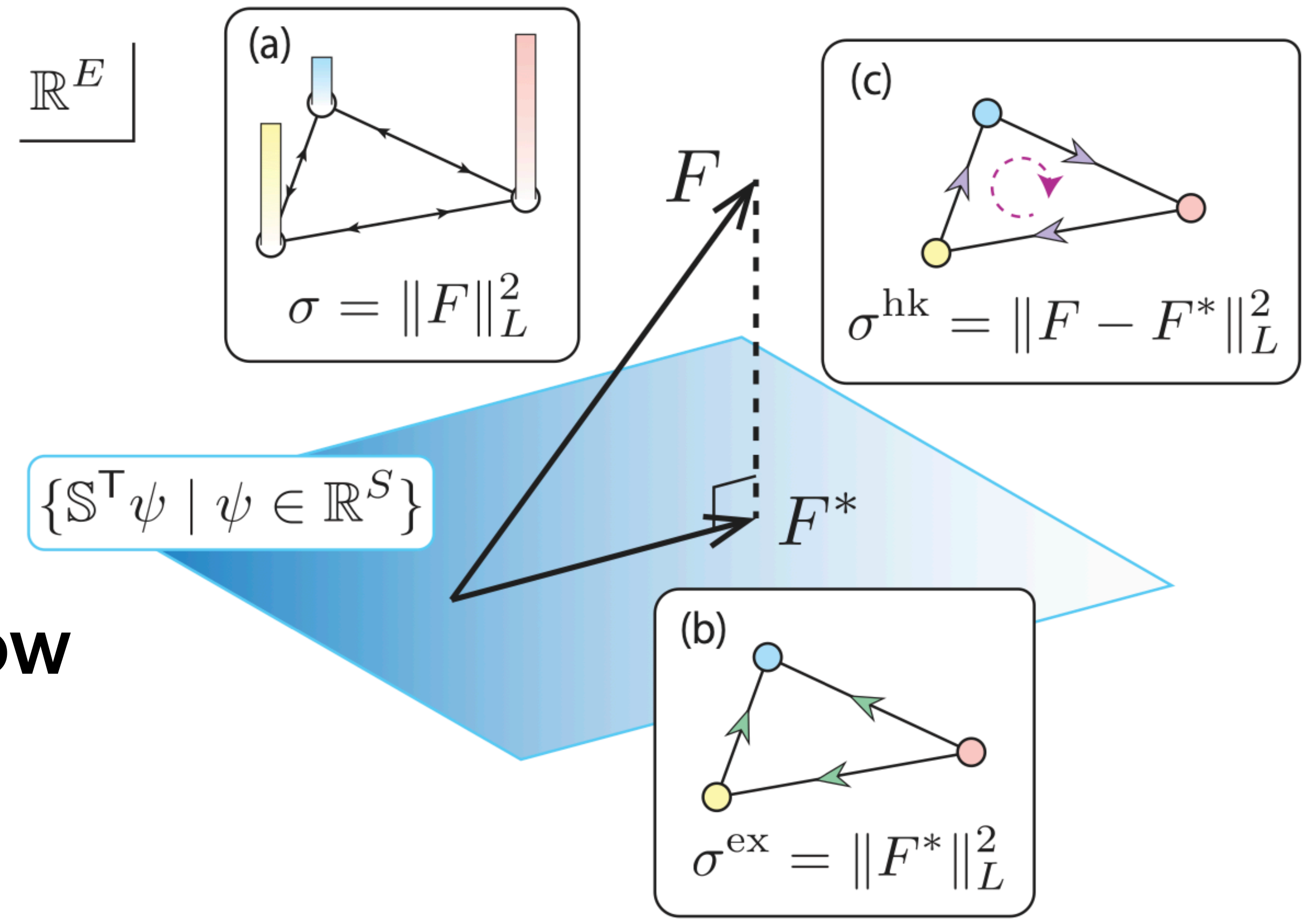
Master equation (or deterministic rate equation)

$$\frac{dp_i}{dt} = \sum_{\rho,\rho'} \mathbb{S}_{i\rho} L_{\rho\rho'} F_{\rho'}$$

$\mathbb{S}_{i\rho}$:Incidence matrix (or stoichiometric matrix)

$L_{\rho\rho'} := \delta_{\rho\rho'} J_\rho / F_\rho$:Edgewise Onsager coefficient

F_ρ :Thermodynamic force J_ρ :Thermodynamic flow



Main idea $\mathbb{S}_{i\rho}$ corresponds to the del operator ∇

Decomposition of force $F_\rho = \sum_i \mathbb{S}_{i\rho}\psi_i + F_\rho^{\mathrm{nc}}$ $\quad F_\rho^{\mathrm{nc}} \in \mathrm{Ker}[\mathbb{S}L]$ $\quad \left(\frac{dp_i}{dt} = \sum_{\rho,\rho',j} \mathbb{S}_{i\rho} L_{\rho\rho'} \mathbb{S}_{j\rho'} \psi_j \right)$

Entropy production rate $\sigma = \sum_{\rho,\rho'} F_\rho L_{\rho\rho'} F_{\rho'} := \langle F, F \rangle_L$

Orthogonality $\langle F - \mathbb{S}\psi, \mathbb{S}\psi \rangle_L = 0$

We can discuss the correspondence.
(e.g., A speed limit, a thermodynamic uncertainty relation and optimal protocol to minimizing the entropy production in finite time.)

Summary

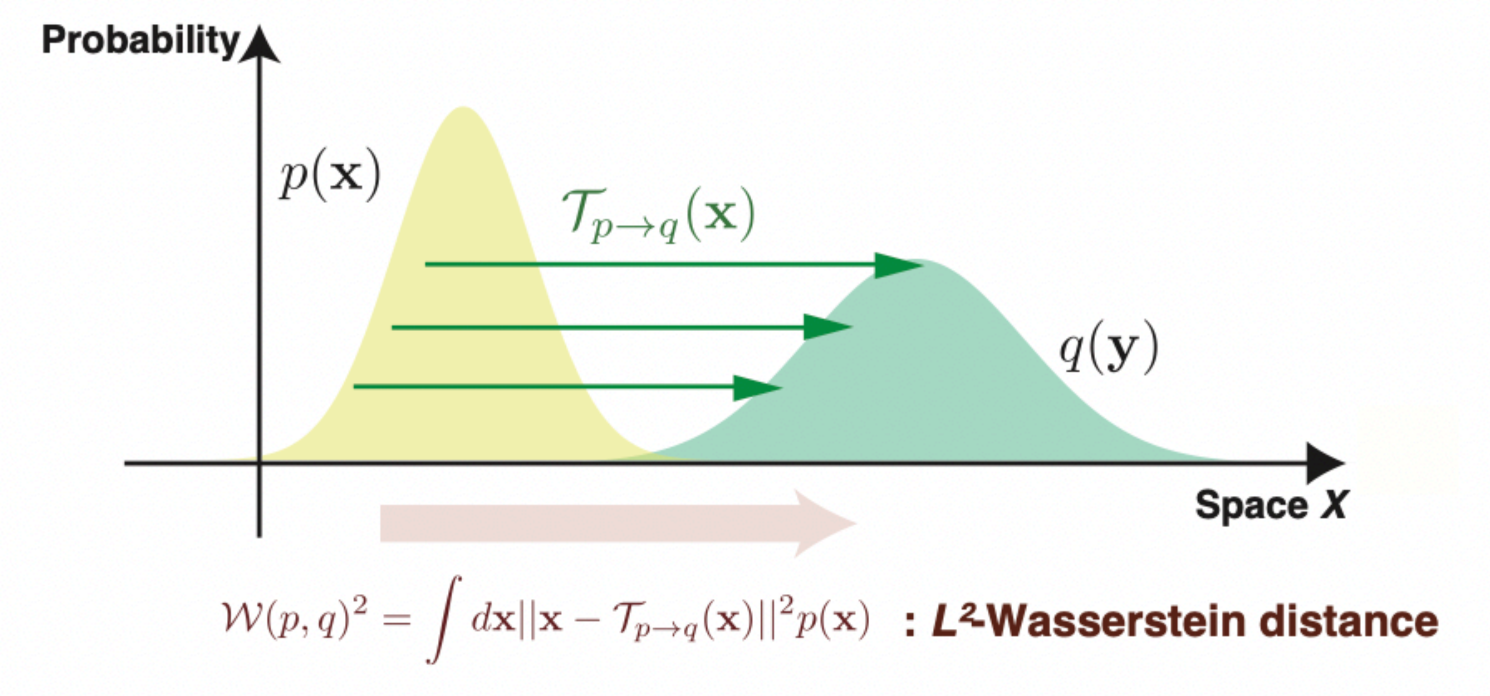
Based on the optimal transport theory, we have constructed a geometric theory of non-equilibrium thermodynamics.

Thermodynamic quantity (Entropy production rate) →

$$\sigma_t \geq \langle \nabla \phi_t, \nabla \phi_t \rangle_{P_t} = \frac{\beta}{\mu} \lim_{\Delta t \to 0} \frac{\mathcal{W}^2(P_t, P_{t+\Delta t})}{(\Delta t)^2}$$

Geometric quantity ← (L2 Wasserstein distance)

Optimal transport



Based on this geometry, we obtain several bounds on the entropy production (a thermodynamic speed limit, a thermodynamic uncertainty relation), an optimal protocol to minimize the entropy production, a decomposition of the entropy production and its variational formulas even for Markov jump process and deterministic rate equation.

Collaborators

Muka Nakazato (Master's degree. in 2021), Andreas Dechant (Kyoto U), Shin-ichi Sasa (Kyoto U), Kohei Yoshimura (D1), Artemy Kolchinsky (Postdoc)

M. Nakazato, and SI. *Physical Review Research* 3, 043093 (2021).
A. Dechant, S-I Sasa, and SI. *Physical Review Research* 4, L012034 (2022).
A. Dechant, S-I Sasa, and SI. *arXiv:2202.04331* (2022).
K. Yoshimura, A. Kolchinsky, A. Dechant, and SI. *arXiv:2205.15227* (2022).