The sub-Riemannian geometry of Optimal Mass Transport

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joint work with

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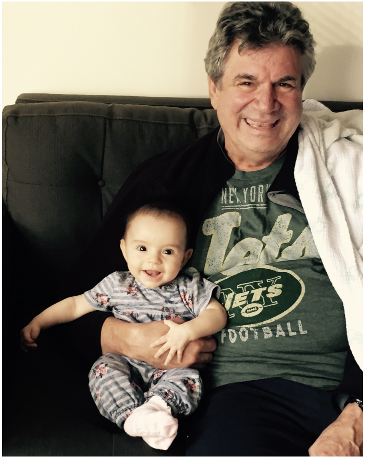
Grant: FA9550-23-1-0096

Controls and Dynamics
Program Review 2024

In loving memory
of our dearest friend and colleague
Allen Tannenbaum
(January 25, 1953 - December 28, 2023)



200y ago till now (Mathematics):

- Optimization - Monge, Kantorovich, Otto, ...
- Large deviations theory - Schrödinger, Cramer, Sanov, ...

Dynamics of ensembles/particle systems

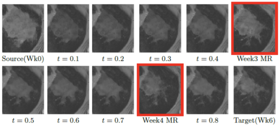
Modern day relevance:

- Computer & biomedical imaging
- Cancer growth models
- Geometry of networks
- Thermodynamics, energy transduction
- Biology, ATPase machine, Flagellar motors
- Uncertainty control & estimation
- Machine learning, ...

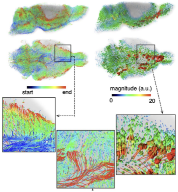
Goals of our program

Stochastic Control and Optimal Mass Trasport - Theory & Applications

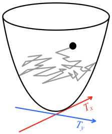
Data augmentation:

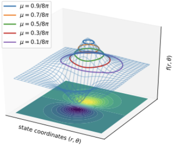


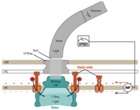
OMT flows:
fluid flows in the brain



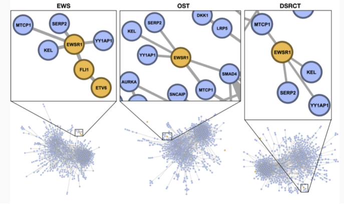
Stochastic engines:
Brownian gyrators



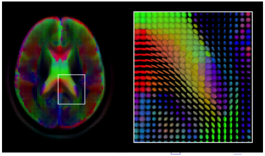




Robustness: gene networks
pathways, hubs, drug response



Matrix OMT:
DTI
Quantum, non-commutative transport



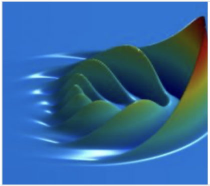
Non-commutative transport

in Spring 2025

Workshop I: Optimal Transport for Density Operators: Theory and Numerics

Part of the Long Program: Non-commutative Optimal Transport

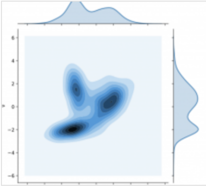
March 31 - April 4, 2025



Workshop II: Dynamics of Density Operators

Part of the Long Program: Non-commutative Optimal Transport

April 28 - May 2, 2025



Workshop III: Statistical and Numerical Methods for Non-commutative Optimal Transport

Part of the Long Program: Non-commutative Optimal Transport

May 19 - 23, 2025

Goals of our program

Stochastic Control and Optimal Mass Trasport - Theory & Applications

Previous reporting:	OMT & thermal/chemical engines
	Applications to Cancer & Biomed
	Sign-indefinite OMT: promotion/inhibition gene regulatory networks

2024

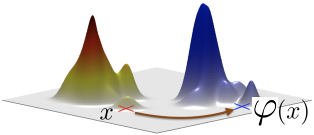
Computational Mathematics	Transport between spatio-temporal marginals
Dynamical Systems and Control Theory	**Sub-Riemannian geometry of OMT** **The isoholonomic problem**

Optimal transport

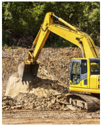
cost $c(x, T(x)) = \|T(x) - x\|^2 \Rightarrow W_2^2(\mu, \nu)$

$$W_2(\mu_0, \mu_1)^2 = \begin{cases} \min_{\mu, u} \int_0^1 \int_X \mu_t \|u\|^2 dxdt \\ \\ \partial_t \mu_t + \nabla \cdot (\mu_t u) = 0 \\ \text{given } \mu_0, \mu_1 \end{cases}$$

$$\inf_{\varphi_\sharp \mu = \nu} \int_\Omega c(x, \varphi(x)) \mu(dx)$$



$$\Rightarrow \begin{cases} \varphi^\star(x) = \nabla \phi(x) \\ \mu_t = (\varphi_t)\sharp \mu_0 \\ \varphi_t = (1-t)\,\mathrm{Id} + t\,\varphi^\star \end{cases}$$



Riemannian geometry of optimal transport

space of densities $\mathcal{D} := \{\mu \geq 0 : \int \mu = 1\}$
tangent space $\mathrm{Tangent}_\mu \cong \{\delta : \int \delta = 0\}$

$\mathrm{Tangent}_\mu \ni \delta \longleftrightarrow u = \nabla\phi$ via

$$\delta + \nabla \cdot (\mu \nabla \phi) = 0$$

Riemannian structure

$$\langle \delta_1, \delta_2 \rangle_\mu := \int \mu \langle \nabla\phi_1, \nabla\phi_2 \rangle dx$$

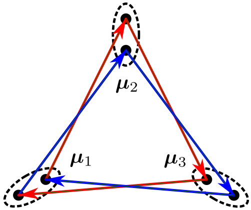
Geodesic distance

$$W_2(\mu_0, \mu_1) = \inf_\mu \int_0^1 \sqrt{\left\langle \frac{\partial\mu}{\partial t}, \frac{\partial\mu}{\partial t} \right\rangle_{\mu(t)}} dt$$

Our starting point

transport of discrete masses

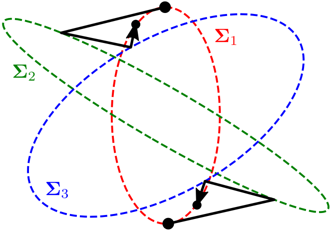
$$\varphi := \varphi^{\star}_{3\mapsto 1} \circ \varphi^{\star}_{2\mapsto 3} \circ \varphi^{\star}_{1\mapsto 2}$$



Our starting point

transport of Gaussians

$$\varphi := \varphi^{\star}_{3\mapsto 1} \circ \varphi^{\star}_{2\mapsto 3} \circ \varphi^{\star}_{1\mapsto 2}$$



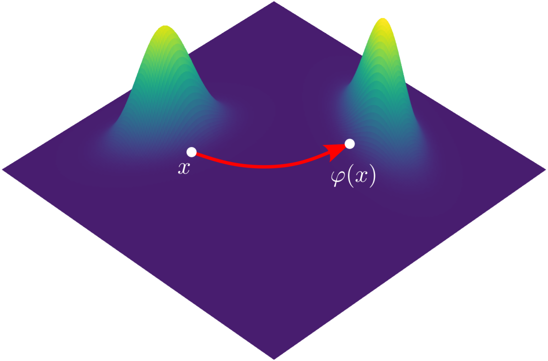
transport of Gaussian distributions

ensembles – linear dynamics

$$\dot{X}_t = -\nabla\phi_t(X_t) =: u_t$$
$$= A_t X_t + r_t$$

$$\phi_t(x) = -\frac{1}{2}x^\intercal A_t x - r_t x$$

$$\dot{\bar{X}}_t = A_t \bar{X}_t + r_t$$



transport of Gaussian distributions

ensembles – linear dynamics

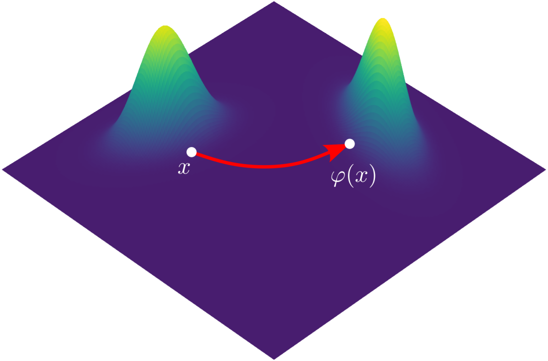
$$\bar{X}_t = 0 \text{ and } \Sigma_t = \mathbb{E}\{X_t X_t^\intercal\}$$

$$\dot{\Sigma}_t = A_t \Sigma_t + \Sigma_t A_t^\intercal$$

$$\dot{\Phi}_t = A_t \Phi_t, \quad \Phi_0 = I$$

$$\mu(x) = \frac{\exp\left(-\frac{1}{2} x^\intercal \Sigma^{-1} x\right)}{\sqrt{(2\pi)^n \det(\Sigma)}}$$

$$\Sigma \in \mathrm{Sym}^+(n)$$



transport of Gaussian distributions

$\mu_0, \mu_1 \in \mathcal{N}(\mathbb{R}^n)$, Σ_0, Σ_1

$$\varphi^\star(x) = \Phi^\star x$$

$$\Phi^\star = \Sigma_0^{-\frac{1}{2}} \left(\Sigma_0^{\frac{1}{2}} \Sigma_1 \Sigma_0^{\frac{1}{2}}\right)^{\frac{1}{2}} \Sigma_0^{-\frac{1}{2}}$$

$$\mathcal{W}_2(\mu_0, \mu_1) = \mathrm{Tr}(\Sigma_0 + \Sigma_1 - 2(\Sigma_0^{\frac{1}{2}} \Sigma_1 \Sigma_0^{\frac{1}{2}})^{\frac{1}{2}}).$$

transport of Gaussian distributions

McCann geodesics

$$\mu_t(x) = (\varphi_t)\sharp\mu_0 \quad = \frac{\exp\left(-\frac{1}{2}x^\intercal\Sigma_t^{-1}x\right)}{\sqrt{(2\pi)^n \det(\Sigma_t)}},$$

remains in $\mathcal{N}(\mathbb{R}^n)$ for $t \in [0,1]$ but not $\mathbb{R}$

$\varphi_t(x) = ((1-t)I + \Phi^\star)x$
$\Sigma_t = ((1-t)I + t\Phi^\star)\sharp\Sigma_0$ with $\Phi\sharp\Sigma = \Phi\Sigma\Phi^\intercal$
Σ_t obeys a Lyapunov equation with

$$A_t = (\Phi^\star - I)(I + t(\Phi^\star - I))^{-1}$$

Wasserstein triangle

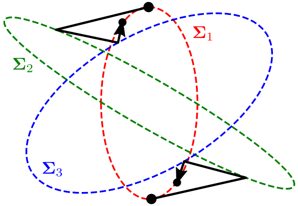
non-commutativity of Monge maps, mixing

$$\Sigma_t := \begin{cases} (I + 3t(\Phi^\star_{1\mapsto 2} - I))\sharp \mathbf{\Sigma}_1 \\ (I + 3(t - \frac{1}{3})(\Phi^\star_{2\mapsto 3} - I))\sharp \mathbf{\Sigma}_2 \\ (I + 3(t - \frac{2}{3})(\Phi^\star_{3\mapsto 1} - I))\sharp \mathbf{\Sigma}_3 \end{cases}$$

$\Phi^\star_{1\mapsto 2}, \Phi^\star_{2\mapsto 3}, \Phi^\star_{3\mapsto 1}$
$\Sigma_1 = \Sigma_0 = \mathbf{\Sigma}_1$

$$\Theta = \Phi^\star_{3\mapsto 1}\Phi^\star_{2\mapsto 3}\Phi^\star_{1\mapsto 2}$$

$$\Theta\sharp\mathbf{\Sigma}_1 = \mathbf{\Sigma}_1$$



Principal Bundle Structure

$\varphi(x) = \Phi x$
$L_\Phi : \Sigma \mapsto \Phi\sharp\Sigma = \Phi\Sigma\Phi^T$

$\Sigma_{\text{ref}} \in \text{Sym}^+(n)$

The OMT principal bundle

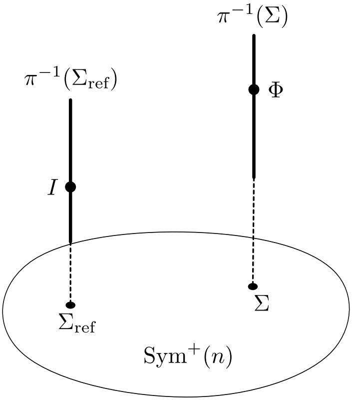
$$\begin{aligned} \pi \;:\; \text{GL}^+(n) &\to \text{Sym}^+(n) \\ \Phi \quad &\mapsto L_\Phi(\Sigma_{\text{ref}}) \end{aligned}$$

Fibers: $\pi^{-1}(\Sigma)$

$\pi^{-1}(\Sigma_{\text{ref}})$ = *isotropy group* of Σ_{ref}

$$\text{SO}(n, \Sigma_{\text{ref}}) = \{\Theta \in \text{GL}^+(n) \mid L_\Theta(\Sigma_{\text{ref}}) = \Sigma_{\text{ref}}\}.$$

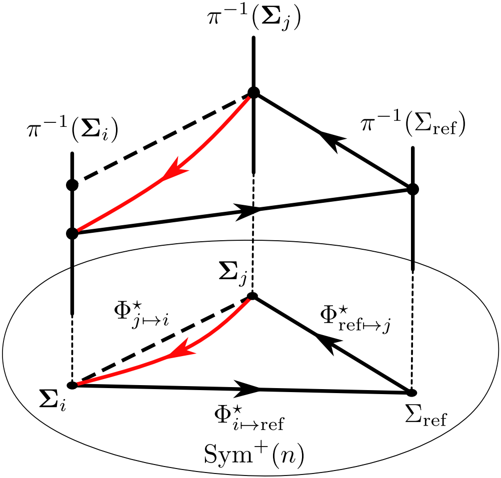
$\text{Sym}^+(n) \simeq \text{GL}^+(n)/\text{SO}(n, \Sigma_{\text{ref}})$



The principal bundle in a nutshell

$\Phi \in \pi^{-1}(\Sigma)$

$$\Sigma = \Phi \Sigma_{\text{ref}} \Phi^T$$



Principal Ehresmann connection

Vertical sub-bundle

$$\mathrm{Ver}_\Phi := \mathrm{Ker}(\mathrm{d}\pi_\Phi) = \{\dot\Phi \in T_\Phi \mathrm{GL}^+(n) \mid \mathrm{d}\pi_\Phi(\dot\Phi) = 0\}.$$

Principal Ehresmann connection: choice of horizontal sub-bundle

1. $T_\Phi \mathrm{GL}^+(n) = \mathrm{Ver}_\Phi \oplus \mathrm{Hor}_\Phi$,
2. $\mathrm{Hor}_{\Phi\Theta} = (R_\Theta)_* \mathrm{Hor}_\Phi$.

Horizontal sub-bundle

$$\mathrm{Hor}_\Phi = \{\dot\Phi \in T_\Phi \mathrm{GL}^+(n) \mid \dot\Phi\Phi^{-1} \in \mathrm{Sym}(n)\}.$$

Transition from Φ_t to Φ_{t+dt} is a Monge map $\iff$ A_t symmetric

Horizontal lift

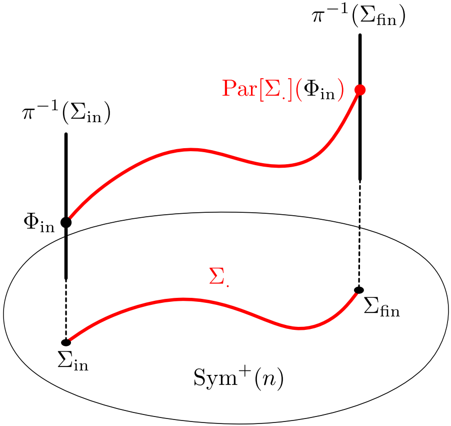
$\Sigma_. : [0,1] \to \mathrm{Sym}^+(n)$ be a $\mathcal{C}^1$ curve,
$A_t = \int_0^\infty e^{-\tau\Sigma_t}\dot\Sigma_t e^{-\tau\Sigma_t} d\tau =: \mathcal{L}_\Sigma(\dot\Sigma)$

$$\dot\Phi_t = A_t\Phi_t, \text{ with } \Phi_0 = \Phi_{in}$$

Parallel transport along Wasserstein curves

Morphism of fibers $\sim$ parallel transport

$$\pi^{-1}(\Sigma_0) \to \pi^{-1}(\Sigma_1) \quad : \quad \Phi \mapsto \mathrm{Par}(\Phi)$$



Complete controllability

There exists a horizontal curve $\Phi_\cdot : [0,1] \to \mathrm{GL}^+(n)$ such that $\Phi_0 = \Phi_{\mathrm{in}}$ and $\Phi_1 = \Phi_{\mathrm{fin}}$, for every $\Phi_{\mathrm{in}}, \Phi_{\mathrm{fin}} \in \mathrm{GL}^+(n)$.

Holonomy group $= \mathrm{SO}(n, \Sigma_{\mathrm{ref}})$: rotations by composing Monge maps.

Sub-Riemannian Metric

$$\mathcal{G}_\Phi(\dot\Phi_1, \dot\Phi_2) = \mathrm{Tr}(\dot\Phi \Sigma_{\mathrm{ref}} \dot\Phi^\intercal)$$

$$d_{SR}(\Phi_0, \Phi_1)^2 = \inf \int_0^1 \mathcal{G}_{\Phi_t}(\dot\Phi_t, \dot\Phi_t)\,\mathrm{d}t = \inf \int_0^1 \mathrm{Tr}\left(A_t \Sigma_t A_t\right)\,\mathrm{d}t.$$

$$\langle \dot\mu_t, \dot\mu_t \rangle = \mathrm{Tr}\left(A_t \Sigma_t A_t\right) = \mathrm{Tr}(\mathcal{L}_{\Sigma_t}(\dot\Sigma_t)\Sigma_t \mathcal{L}_{\Sigma_t}(\dot\Sigma_t))$$

Wasserstein-Otto metric on the base space

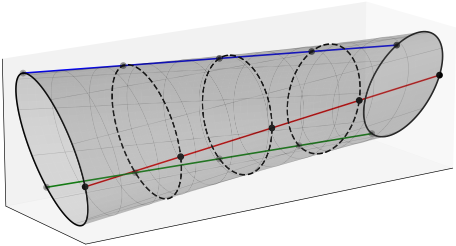
Isoparallel Mass Transport

Σ_{in}, Σ_{fin} in $\text{Sym}^+(n)$
Φ_{des} in $\text{GL}^+(n)$ with $\Phi_{\text{des}} \sharp \Sigma_{\text{in}} = \Sigma_{\text{fin}}$

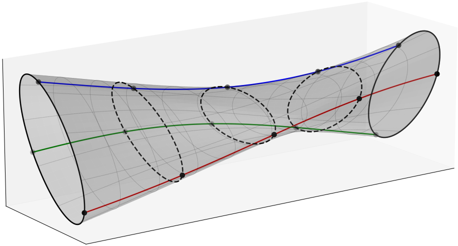
find a curve $\Sigma_.$ of minimal length s.t.,
$\Sigma_0 = \Sigma_{\text{in}}$, $\Sigma_1 = \Sigma_{\text{fin}}$, and

$$\text{Par}[\Sigma_.] = \Phi_{\text{des}}$$

In the base space of Σ's

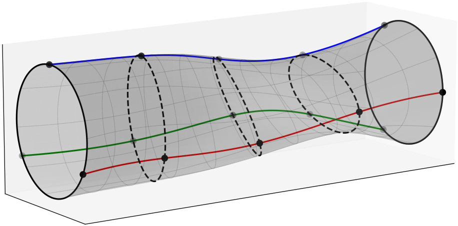


Tracer particles traversing McCann geodesic



Tracer particles traversing isoparallel curve

Rotation in the base space of Σ's

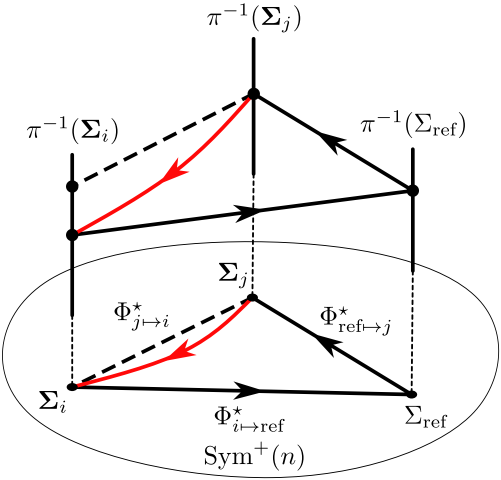


Tracer particles traversing the isoholonomic curve connecting $\Sigma_{\text{in}} = I$, $\Sigma_{\text{fin}} = I$

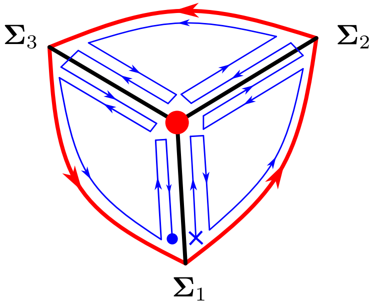
multiagent and particle systems
path planning, uncertainty control, mixing, registration

the holonomy of the loop,
may not be trivial

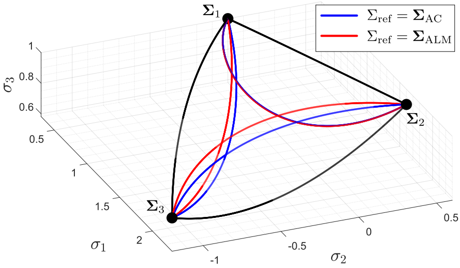
$$\boldsymbol{\mu}_i \xrightarrow{\varphi^\star_{i\mapsto \mathrm{ref}}} \mu_{\mathrm{ref}} \xrightarrow{\varphi^\star_{\mathrm{ref}\mapsto j}} \boldsymbol{\mu}_j$$



multiagent and particle systems
path planning, uncertainty control, mixing
registration $\Leftarrow$



McCann geodesics (black)
Identical holonomy as a function of reference (blue, red).



Recap

the principal bundle structure encodes particle location

Lagrangian viewpoint to OMT
trajectories and mixing are of interest
holonomy of trajectories

Key insights:
Eulerian constraint on velocity=potential via Ehresmann connection
sub-Riemannian structure by this connection - Wasserstein-Otto metric

Applications and future directions:
modeling flow based on aggregate information
and/or location of tracer particles
estimate the holonomy of transport
Ehresmann connection/nature of forces
what about stochastic excitation?...

Mahmoud Abdelgalil

Thank you for your attention

Sub-Riemannian Geometry, Mixing, and the Holonomy of OMT
M. Abdelgalil and T.T. Georgiou, https://arxiv.org/abs/2408.14707

Thanks to AFOSR

University of California, Irvine