Optimal transportation, Action principle and Dynamics

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Abstract

The problem of optimal transportation was proposed my Monge in 1781. It became very popular in the last decades, since the pioneering monograph of Yan Brenier in 1987 on vector rearrangements. Since then, a long list of authors found beautiful connections between this concept and various fields in mathematics, such as PDE, probability, fluid dynamics, geometry and functional analysis. In this talk I'll consider optimal transportation as an extended Lagrangian formalism and discuss some aspects of dynamics which are naturally related to this point of view.

Overview

- Some fundamental problems in a nutshell
- The Monge problem and Kantorovich relaxation
- Dual formulation
- Extended Lagrangians
- Applications:

  (I) Circle maps and rotation numbers

  (II) Steady flow, optimal networks

  (III) Dynamics of adhesive particles

Let $\rho(x,t)$ be a density of a cloud in a domain Ω,

$$\int_\Omega \rho(x,t)dx = 1 \ .$$

Can we identify the particle's velocities?

Look for a velocity field $\vec{v}(x,t)$ so that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \ .$$

Can $\vec{v}$ be determined? Is it unique?

If $\vec{v}_0$ is determined and $\vec{\zeta}$ is a free divergence vector field supported on Ω, then

$$\vec{v}(x,t) = \vec{v}_0(x,t) + \frac{\vec{\zeta}(x,t)}{\rho(x,t)}$$

is also a transporting field.

Helhmoltz Decomposition: If $\rho > 0$ on a compact manifold Ω, then any field $\vec{v}$ on Ω can be decomposed as

$$\vec{v} = \nabla \phi + \frac{\vec{\zeta}}{\rho} \ \ ; \ \ \nabla \cdot \vec{\zeta} = 0 \ .$$

Does ϕ exists? Attempt to solve the equation for ϕ

$$\nabla \cdot (\rho \nabla \phi) = -\frac{\partial \rho}{\partial t}$$

for any t on Ω.

This is elliptic equation (and solvable) only if $\rho > 0$ and smooth enough on Ω.

Can we identify a unique velocity field $\vec{v}$ if the density $\rho(x,t)$ is extended to an orbit of measures $\mu_{(t)}(dx)$, such as

$$\mu_{(t)}(dx) = \sum m_i(t) \delta_{X_i(t)}$$

where $\sum m_i(t) = 1$ and $X_i(\cdot) : \mathbb{R} \to \Omega$ are continuous orbits?

To avoid problems at infinity, we assume that Ω is a compact manifold. For example, the flat torus in $\mathbb{R}^k$.

. A fundamental problem:

Given a density field $\rho(x,t)$ of a cloud on $\Omega \times [0,1]$, which assumptions would guarantee a unique velocity field $\vec{v}$ which transports ρ so that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \ .$$

Also, what is the pressure field acting on the cloud:

$$\nabla P = \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} \quad ?$$

"Inverse" problem

Given a pair of densities $\rho_0(x)$, $\rho_1(x)$ and a prescribed pressure field $P = P(x,t)$, is it possible to find a unique pair $\rho(x,t)$, $\vec{v}(x,t)$ verifying

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad ; \quad \frac{\partial \vec{v}}{\partial t} + \vec{v} \cdot \nabla \vec{v} = \nabla P$$

subjected to the end conditions

$$\rho(x,0) = \rho_0(x) \quad ; \quad \rho(x,1) = \rho_1(x) \ ?$$

The Monge problem(1781)

Given μ_0, μ_1 a pair of probability Borel measure on Ω (metric space).

A Borel map T *push forward* μ_0 to μ_1:

$$T_{\#}\mu_0 = \mu_1 \iff \mu_0\left(T^{-1}(\mathcal{A})\right) = \mu_1(\mathcal{A}) \ \ \forall \mathcal{A} \in \sigma(\Omega) \ .$$

Equivalently,

$$\int_\Omega \phi(T(x))\mu_0(dx) = \int_\Omega \phi(x)\mu_1(dx) \ \ \forall \phi \in C_0(\Omega) \ .$$

Given a cost function $c : \Omega \times \Omega \to \mathbb{R}$, the Monge problem is

$$M := \min_{T_{\#}\mu_0=\mu_1} \int_\Omega c(x, T(x))\mu_0(dx) \ . \qquad (\mathbf{M})$$

Remark: If μ_0 contains an atom, then there is, in general, no mapping T which pushes μ_0 to μ_1.

Kantorovich relaxation (1942)

$$K := \inf_{\lambda} \int\int c(x,y)\lambda(dx,dy) \quad ; \; \pi^{(0)}_{\#}\lambda = \mu_0 \; , \; \pi^{(1)}_{\#}\lambda = \mu_1 \qquad (\mathbf{K})$$

Here $\pi^{(i)}, i = 0, 1$ are the natural projections of $\Omega \times \Omega$ on its factors.

Compactness of C^* implies the existence of a minimizer of **(K)**.

The condition $\pi^{(0)}_{\#}\lambda = \mu_0 \; , \; \pi^{(1)}_{\#}\lambda = \mu_1$ is equivalent to

$$\int_\Omega \int_\Omega (\phi(x) - \psi(y))\lambda(dxdy) = \int_\Omega \phi(x)\mu_0(dx) - \int_\Omega \psi(x)\mu_1(dx) \; .$$

(**K**) is reduced to (**M**) if the minimizer is attained at

$$\lambda = \delta_{y-T(x)}\mu_0(dx) \; .$$

Therefore

$$K \le M \; .$$

Surprising result: If μ_0 has no atoms, then $K = M$ (Ambrosio)

Examples: Discrete cases

Let $x_1, \ldots x_N \in \Omega$, $y_1, \ldots y_N \in \Omega$. Let $C_{i,j} := c(x_i, y_j)$. For

$$\mu_0 = \frac{1}{N}\sum_1^N \delta_{x_i} \ , \quad \mu_1 = \frac{1}{N}\sum_1^N \delta_{y_i}$$

we get the marriage problem:

$$M = \min_{T \in S_N} \sum_{i=1}^N C_{i,T(i)} \ .$$

Kanterovich: If

$$\mu_0 = \sum_1^N \alpha_i \delta_{x_i} \ , \quad \mu_1 = \sum_1^N \beta_i \delta_{y_i}$$

where $\alpha_1, \beta_i > 0$, $\sum_1^N \alpha_i = \sum_1^N \beta_i = 1$ then

$$K(\mu_0, \mu_1) = \inf_{\lambda \in \Gamma} \left\{ \sum_{i=1}^N \sum_{j=1}^N \lambda_{i,j} C_{i,j} \ ; \ \Gamma := (\lambda)_{i,j} \geq 0 \ , \ \sum_i \lambda_{i,j} = \beta_j , \ \sum_j \lambda_{i,j} = \alpha_i \ . \right\}$$

Birkhoff Theorem: If $\alpha_i = \beta_i = 1/N$ for $1 \leq i \leq N$ then all the extreme points of Γ are permutation matrices.

Conclusion: In the case of the marriage problem $M = K$.

Dual formulation

Given

$$\Gamma^{:} = \{\phi, \psi \in Lip(\Omega) \ ; \ \phi(x) - \psi(y) \leq c(x, y) \ \forall x, y \in \Omega\}$$

The dual formulation is:

$$E = \max_{\phi, \psi \in \Gamma^*} \int_\Omega \phi(x)\mu_0(dx) - \psi(x)\mu_1(dx) \qquad (E) \ .$$

So:

$$\int_\Omega \phi(x)\mu_0(dx) - \psi(x)\mu_1(dx) = \int_\Omega \int_\Omega (\phi(x) - \psi(y))\lambda(dxdy)$$
$$\leq \int_\Omega \int_\Omega c(x, y)\lambda(dxdy) \ .$$

In particular

$$E \leq K \leq M \ .$$

If μ_0 has no atoms there is an equality $E = M$.

In particular, $\phi(x) - \psi(y) = c(x,y)$ in the support of the optimal measure and $\phi(x) - \psi(T(x)) = c(x,T(x)) \leq c(x,y) \;\; \forall \, y \in \Omega \, , x \in Supp(\mu_0)$. So

$$\nabla\psi \circ T = -\nabla_y c(x,T(x)) \;\; ; \;\; \nabla\phi = \nabla_x c(x,T(x)) \; .$$

Special case: Quadratic cost $c(x,y) = |x-y|^2/2$. Then the optimal map satisfies

$$T(x) = x - \nabla\phi(x) = \nabla\left(\frac{x^2}{2} - \phi(x)\right) \equiv \nabla\Phi(x) \; .$$

Φ is a convex function. Indeed, the optimal pair satisfies

$$\phi(x) = \min_y \{\psi(y) + c(x,y)\} = \frac{x^2}{2} + \min_y \left\{\psi(y) + \frac{y^2}{2} - x\cdot y\right\} \;\; ; \quad .$$
$$= \frac{x^2}{2} - \Psi^*(x)$$

where $\Psi(y) = \frac{y^2}{2} + \psi(y)$.

Brenier: Any mapping $T : \Omega \to \Omega$ has a convex representation. There exists convex Φ and a map $S_{\#}\mu_0 = \mu_0$ so that $T = \nabla\Phi \circ S$. The only optimal map is $T = \nabla\Phi$.

This result is generalized for any *convex*, homogeneous cost $c(x,y) = c(|x-y|)$.

Another aspect: McCann interpolation

$$\mu_t = T^{(t)}_{\#}\mu_0$$

where

$$T^{(t)}(x) = (1-t)x + t\nabla\Phi \ .$$

Orbits of McCann interpolation never intersect!

$$T^{(t)}(x) = T^{(t)}(y) \Longrightarrow \nabla\Phi(x) - \nabla\Phi(y) = -\frac{1-t}{t}(x-y) \Longrightarrow (\nabla\Phi(x) - \nabla\Phi(y))\cdot(x-y) < 0 \ .$$

$T^{(t)}$ is an optimal map for the quadratic transport from μ_0 to μ_t:

$$T^{(t)}(x) = \nabla\left(\frac{(1-t)x^2}{2} + t\Phi(x)\right)$$

and $M(\mu_0, \mu_t) := \int_\Omega |T^{(t)}(x) - x|^2 \mu_0(dx) = t\int_\Omega |\nabla\phi(x)|^2 \mu_0(dx)$.

Extended Lagrangian formulation

Assume that the distribution of particles at time t is given by a positive measure $\mu_{(t)}$ on Ω. We usually denote a trajectory of probability measures $\mu_{(t)}$, $0 \leq t \leq T$ by μ. We denote the set $\mathbf{H}_2[0,T]$ as all such trajectories for which

$$\|\mu\|^2_{2,T} := \inf_{\vec{E}} \int_0^T \left| \frac{d\vec{E}_{(t)}}{d\mu_{(t)}} \right|^2 \mu_{(t)}(dx)dt < \infty \qquad (*)$$

$$\frac{\partial \mu}{\partial t} + \nabla_x \cdot \vec{E}_{(t)} = 0$$

in the sense of distributions.

Some properties of $\mathbf{H}_2$:

Proposition: If $\mu \in \mathbf{H}_2$ then $t \to \mu_{(t)}$ is Holder 1/2 in the C^* topology equipped with the norm

$$d(\mu_1, \mu_2) := \sup_{|\nabla \phi| \leq 1} \int_\Omega \phi(x) \left(\mu_1(dx) - \mu_2(dx)\right) \ .$$

The Kantorovich problem (quadratic cost):

$$K(\mu_0, \mu_1) = T^{-1} \inf \left\{ \|\mu\|^2_{2,T} \ ; \ \mu \in \mathbf{H}_{2,T}, \ \mu_{(0)} = \mu_0, \ \mu_{(T)} = \mu_1 \ . \right\}$$

Examples:

- If $\mu_{(t)}$ have a density $\rho = \rho(x,t)$ then $d\vec{E}_{(t)}/d\mu_{(t)} := \vec{u}(x,t)$ is a velocity field and

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \ , \ \|\mu\|^2_{2,T} = \int_0^T \int_\Omega \rho(x,t)|\vec{u}|^2(x,t)dxdt \ .$$

- If $\mu_{(t)} = \delta_{X(t)}$ where $X \in C^1$ then

$$\vec{E}_{(t)} = \dot{X}(t)\delta_{X(t)} \ , \ \|\mu\|^2_{2,T} = \int_0^T |\dot{X}|^2 dt \ .$$

- If $\mu_{(t)} = \sum_i m_i(t)\delta_{X_i(t)}$ where $X_i \in C^1$, $m_i(t) \geq 0$, $\sum_i m_i(t) = 1$, then $\mu \in \mathbf{H}_{2,T}$ if $\dot{m}_i(t) = 0$ whenever $m_i(t) \neq m_j(t)$ for any $i \neq j$. In this case $\|\mu\|^2_{2,T} = \sum_i \int_0^T m_i(t)|\dot{X}(t)|^2 dt$.

Application to circle maps:

Let $\Omega = \mathbb{S}^1$ and $\mu_{(t)} := \mu_{(t+1)}$. Identify $\mathbb{S}^1$ with $\mathbb{R} mod 1$. If there exists a velocity field $u(x,t)$ on $\mathbb{S}^1 \times \mathbb{S}^1$, let

$$\dot{x} = u(x,t) \ .$$

The rotation number is defined by $r = \lim_{t\to\infty} \frac{x(t)}{t}$.

Theorem: If $\mu \in \mathbf{H}_2$ is a circle map, then the rotation number exists. It is also possible to define a strong topology on $\mu \in \mathbf{H}_2$ for which the rotation number is Lipshitz continuous.

Examples:

- $\mu_{(t)}(dx) = \delta_{X(t)}$ where $X(t) \in C^1(\mathbb{S}^1)$. $X(t+1) = X(t) + d \quad \forall t \in \mathbb{R}$ where $d := Deg(X) \in \mathbb{Z}$. Then $r = d$.
- Mixture: $\mu_{(t)} = \sum_1^N \beta_i \delta_{X_i(t)}$, $\sum \beta_i = 1$. Then $r = \sum \beta_i Deg(X_i)$.
- Rigid orbits: $\mu_{(t)}(dx) = g(x - X(t))dx$. $r = Deg(X)\left(1 - \frac{1}{\int_{\mathbb{S}^1} g^{-1} dx}\right)$.

For a given pair of probability measures μ_0, μ_1, the *extended action principle* is defined by

$$A(\mu_0, \mu_1) := \min_{\mu} \frac{1}{2} \|\mu\|^2_{2,T} \quad ; \quad \mu_{(0)} = \mu_0, \ \mu_{(T)} = \mu_1 \ .$$

Benamou and Brenir

If $\mu_0 = \rho_0 dx, \mu_1 = \rho_1 dx$ are "smooth enough" then $A(\mu_0, \mu_1)$ is the the Monge optimal for the transport $\mu_0 \to \mu_1$ for quadratic cost. Moreover, the velocity field $\vec{u}$ verifying

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0$$

defines the optimal map:

$$\dot{x} = \vec{u}(x, t) \ , x(0) = x \implies T(x) = x(T) \ .$$

Extended action subjected to a prescribed pressure:

The extended Lagrangian with a prescribed pressure P and end conditions:

$$A_{P,T}(\mu_0, \mu_1) = \inf_{\mu_{(\cdot)} \in \Gamma(\mu_0,\mu_1)} \left[\frac{1}{2} \|\mu\|_{2,T}^2 - \int_0^T \int_\Omega P(x,t) \mu_{(t)}(dx) dt \right] .$$

where

$$\Gamma(\mu_0, \mu_1) := \left\{ \mu_{(\cdot)} \in \mathbf{H}_2, \quad , \quad \mu_{(0)} = \mu_0 \quad ; \quad \mu_{(T)} = \mu_1 \ . \right\}$$

The associated Hamilton-Jacobi equation

$$\frac{\partial \phi}{\partial t} + \frac{1}{2} |\nabla_x \phi|^2 + P = 0 \quad ; \quad (x,t) \in \Omega \times (0,T) \ ,$$

and the continuity equation

$$\frac{\partial \mu_{(t)}}{\partial t} + \nabla_x \cdot \left(\mu_{(t)} \nabla_x \phi \right) = 0 \ .$$

Theorem: For any pair of end conditions μ_0, μ_1 there exists an orbit $\mu \in \mathbf{H}_2([0,T])$ which realizes the infimum of $A_{P,T}$.

Some definitions:

The cost function:

$$C_P(x,y,\tau,t) := \min \left\{ \int_\tau^t \left(\frac{|\dot{\overline{x}}|^2}{2} + P(\overline{x}(s),s) \right) ds \quad ; \quad \overline{x} : [\tau,t] \to \Omega \right\}$$

where $\overline{x}(\tau) = y$, $\overline{x}(t) = x$. In particular, if $P = 0$: $C_0(x,y,\tau,t) := \frac{|x-y|^2}{2(t-\tau)}$.

i) A *forward (res. backward)* solution is defined, for $t \in [0,T]$, by

$\overline{\phi}(x,t) := \min_y \{C_P(y,x,0,t) + \phi(y,0)\}$, res. $\underline{\phi}(x,t) := \sup_y \{-C_P(x,y,t,T) + \phi(y,T)\}$.

ii) If $\phi(\cdot,0)$ and $\phi(\cdot,T)$ are Lipschitz on Ω then both $\overline{\phi}$ and $\underline{\phi}$ are Lipschitz on $\Omega \times [0,T]$.

iv) $(\overline{\phi},\underline{\phi})$ is called *a reversible pair* if $\overline{\phi} = \underline{\phi}$ on Ω for $t = 0$ and $t = T$. In this case, $\overline{\phi}(x,t) \geq \underline{\phi}(x,t)$ on $\Omega \times [0,T]$.

v) If $(\overline{\phi},\underline{\phi})$ is a reversible pair, then the *reversibility set* is defined by $K_0(\overline{\phi},\underline{\phi}) := \left\{(x,t) \in \Omega \times (0,T) \ ; \ \overline{\phi}(x,t) = \underline{\phi}(x,t) := \psi(x,t)\right\}$. $\nabla_x \psi(x,t) = \nabla_x \overline{\phi} = \nabla_x \underline{\phi}$ is Lipschitz on the reversibility set. We call ψ a *reversible solution*.

Theorem: [W] If ϕ_0, ϕ_1 maximizes

$$\int_\Omega (\phi_1 \mu_1(dx) - \phi_0 \mu_0(dx))$$

subjected $\phi_1(x) - \phi_0(y) \leq C_P(x, y, 0, T)$ for any $x, y \in \Omega$, then $\{\phi_0, \phi_1\}$ is a reversible pair. The reversibility function ψ verifies the Hamilton-Jacobi equation, and the optimal solution of A_P is supported in $K_0(\phi_0, \phi_1)$ and verifies the continuity equation subjected $\nabla\phi = \nabla\psi$. Moreover, the flow

$$\frac{d\mathbf{T}^{(t,s)}}{dt} = \nabla\psi\left(\mathbf{T}^{(t)}_{(x)}, t\right) \quad ; \quad \mathbf{T}^{(t,t)} := \mathbf{I_d}$$

transports this orbit $\mathbf{T}^{(t,s)}_{\#}\mu_{(s)} = \mu_{(t)}$. The limit $\lim_{t\to T, s\to 0} \mathbf{T}^{(s,t)} := \mathbf{T}$ if exists as a Borel map, verifies

- The particles of the optimal flow subjected to a prescribed pressure do not collide (and, in particular, do not stick).
- There are no shock waves for the Hamilton-Jacobi equation. Indeed, ψ is a reversible solution, as claimed.

Steady flows under prescribed sources and sinks

Let Σ be distributed measure of sources and sinks on Ω.

$$\Sigma = \Sigma_+ - \Sigma_- \quad , \quad \int_\Omega \Sigma^+(dx) = \int_\Omega \Sigma^-(dx)$$

For example:

$$\Sigma_\pm = \sum_1^N \lambda_i^\pm \delta_{x_i^\pm} \ , \ \sum_1^N \lambda_i^+ = \sum_1^N \lambda_i^- := \Lambda \quad , \ \lambda_i^\pm > 0 \ .$$

Define

$$\|\mu\|_{2,T,\Sigma}^2 := \inf_{\vec{E}} \int_0^T \int_\Omega \left| \frac{d\vec{E}}{d\mu_{(t)}} \right|^2 \mu_{(t)}(dx)dt \ ; \ \partial_t \mu + \nabla_x \cdot \overrightarrow{E} = \Sigma \ .$$

Consider

$$A_{P,T,\Sigma}(\mu_0, \mu_1) := \inf_{\mu_{(\cdot)} \in \Gamma(\mu_0,\mu_1)} \left[\frac{1}{2} \|\mu\|_{2,T,\Sigma}^2 - \int_0^T \int_\Omega P(x,t)\mu_{(t)}(dx)dt \right] \ .$$

$$A_{P,\Sigma} := \lim_{T\to\infty} T^{-1} A_{P,T,\Sigma}(\mu_0, \mu_1) \ .$$

In this limit, the end conditions μ_0, μ_1 are "forgotten" and

$$A_{P,\Sigma} = \inf_{\vec{E},\mu} \int_\Omega \left(\frac{1}{2} \left| \frac{d\vec{E}}{d\mu} \right|^2 - P \right) \mu(dx) \quad ; \quad \nabla_x \cdot \overrightarrow{E} = \Sigma \quad .$$

Dual formulation

$$\mathcal{A} = \inf_{\mu} \sup_{\phi \in C_b^1} \left[- \int_\Omega \left[P + \frac{1}{2} |\nabla \phi|^2 \right] \mu(dx) + \int_\Omega \phi \Sigma(dx) \right]$$

$$\overline{P} := \sup_{\Omega} P \quad .$$

For any $E \geq \overline{P}$ the Riemannian (semi-)metric associated with the Maupertuis' action principle

$$d\sigma_E = \sqrt{E - P(x)}d|x| \ , \quad E > \overline{P} \ .$$

The geodesic distance is $D_E(\cdot, \cdot)$. A geodesic arc connecting two point x, y coincides with

$$\ddot{x} + \nabla_x P(x(t)) = 0 \quad x(0) = x_0, \ x(T) = x_1 \ ,$$

corresponding to the energy level $|\dot{x}|^2/2 + P(x) = E$. Here $T = T_{x_0,x_1}(E)$ is the time of flight from x_0 to x_1 (which is, of course, a function of E as well).

$$K_E(\Sigma_+, \Sigma_-) := \sum_{i=1}^{N} \sum_{j=1}^{N} A^E_{i,j} D_E(x_i^+, x_j^-) := \min_{A \in \mathcal{Q}} \sum_{i=1}^{N} \sum_{j=1}^{N} A_{i,j} D_E(x_i, x_j) \ ,$$

$$\mathcal{Q} := \left\{ (A)_{i,j} \geq 0 \ ; \ \sum_{i=1}^{N} A_{i,j} = \lambda_j^- \quad , \quad \sum_{j=1}^{N} A_{i,j} = \lambda_i^+ \ . \right\}$$

Theorem: The minimum of the steady action is

$$\mathcal{A} = \max_{E \geq \overline{P}} \left[\sqrt{2} K_E \left(\Sigma_-, \Sigma_+ \right) - E \right] \ .$$

The optimal $\mu = \mu(dx)$ is supported on the bi-graph $G_{E_0} = \cup_{A^E_{i,j} > 0} L_E(i,j)$ of geodesic curves $L_E(i,j)$ connecting x_i^+ to x_j^- w.r to $d\sigma_E$,

Case a: $E > \overline{P}$. Then there exists an action minimizer supported on the bi-graph G_E so that $\mu \left(L_E(i,j) \right) > 0$ only if $A^E_{i,j} > 0$. To wit:

$$\mu \left(L_E(i,j) \right) = A^E_{i,j} T_{i,j}(E) \ \ ,$$

where $T_{i,j}(E) = T_{x_i,x_j}(E)$.

Case b: Somewhere over the rainbow: If $E = \overline{P}$ is the maximizer of $\mathcal{A}$ then the following holds: Let μ_0 be the measure supported on $G_{\overline{P}}$. Then there exists $\beta \in [0, 1)$ so that

$$\sum_{i=1}^{N} \sum_{j=1}^{N} A_{i,j}^{E} T_{i,j}(E) = 1 - \beta \leq 1 \ .$$

$$\mu = \mu_0 + \beta \delta_{x_0} \quad , \quad P(x_0) = \overline{P} \ .$$

In both cases (a) *and* (b), the following claim is valid:

Time/Flux duality: *The expectation of the inverse flow time,* $\mathbb{E}_\mu \left(T^{-1}\right)$ *equals the total in(out) flux* $\Lambda := \sum_{i=1}^{N} \lambda_i = -\sum_{j=1}^{N} \lambda_j$*:*

$$\mathbb{E}_\mu(T^{-1}) := \sum_{i=1}^{N} \sum_{j=1}^{N} \mu \left(L_{E_0}(i,j)\right) T_{i,j}^{-1}(E) = \Lambda \ .$$

Adhesive particles and optimal mass transportation

(*zero-pressure dynamics*)

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \vec{u}) = 0 \quad ; \quad \frac{\partial (\rho \vec{u})}{\partial t} + \nabla_x \cdot (\rho \vec{u} \otimes \vec{u}) = 0 \ .$$

This system can be viewed as an initial value problem, subjected to

$$\rho(x, 0) = \rho_0(x) \geq 0 \quad , \quad \vec{u}(x, 0) = \vec{u}_0(x) \ .$$

As long as the solution is *classical* (namely, continuously differentiable), the momentum equation can be written as the Burger's equation

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla_x \vec{u} = 0 \ .$$

Zero pressure and dynamics of adhesive particles

- Zeldovich (1970): Sticky particle model.
- Existence: E, Rykov and Sinai (1996) Brenier and Grenier (1998), ect.
- Uniqueness: Bouchut and James (1999)

Non-reversible dynamics (entropy solutions) and singular shock waves.

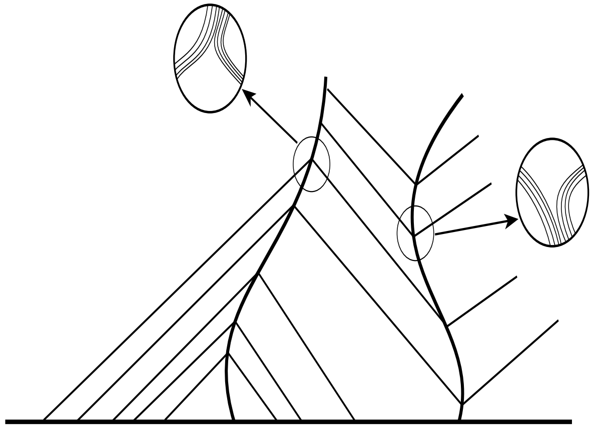
A shock wave can be created out of smooth initial data. Two (or more) shock waves may collide to create a stronger shock. This is COAGULATION.

The arrow of time leads to smaller number of stronger shocks. Colliding particles will never sepatare!

How to model FRAGMENTATION?

Some observations

- Fundamental principles of physics are time reversible. (It is us, the observers, who are, unfortunately, not reversible!)
- Energy is lost in the inelastic collision. Hence, the sticking particle dynamics is not reversible.
- As a result, the solutions of the zero-pressure gas dynamics corresponding to sticking particle are (generalized) entropy solutions: (no refractive shocks, no spontaneous emergence of refractive waves).
- Hence, there are no fragmentation waves!
- The process of fragmentation is currently described by phenomenological kernels. It is based on ad hoc probabilistic assumptions which have nothing to do with the fundamental principle of physics!
- In physics, reversible processes are usually derived from an action principle.



. Resolution of coagulating and fragmenting orbits:

A very strong and short range repulsive force acting when the density is very high.

System of finite number of particles

For an orbit $\vec{x}(t) = (x_1(t), \ldots x_N(t))$ $0 \le t \le T$, the action is

$$A(\vec{x}; T) := \int_0^T L\left(m_1 \dot{x}_1, \ldots m_N \dot{x}_N\right) dt$$

where

$$L(p_1, \ldots p_N) := \sum_1^N \frac{|p_i|^2}{2m_i}$$

and

$$\underline{A}(\vec{x}^{(0)}, \vec{x}^{(1)}; T) :=$$

$$\min_{\vec{x}(\cdot)} \left\{ A(\vec{x}; T) \; ; \; \vec{x}(0) = \vec{x}^{(0)} \; , \vec{x}(T) = \vec{x}^{(1)} \right\} \; .$$

Note that here the masses m_i of the particles are constants.

In order to implement collisions into an action principle, we must introduce inner energy, and allow particles to exchange mass.

State space: Γ is the set of N orbits $(x_i(t), m_i(t))$ so that

a) $x_i \in C([0,T];\Omega)$, $1 \leq i \leq N$.

b) m_i are sequentially constants, so $dm_i/dt = 0$ if $x_i(t) \neq x_j(t)$ for any $i \neq j$.

c) If for $\tau \in (0,T)$ there exists a subset $I \subset \{1, \dots N\}$ for which $x_i(\tau) = x_j(\tau) \equiv x$ for all $i, j \in I$ while $x_l(\tau) \neq x$ for $l \notin I$, then

$$\sum_{i \in I} m_i(t^-) = \sum_{i \in I} m_i(t^+) \ .$$

Inner energy: There is a function $\xi = \xi(m)$, called the inner energy of a particle of mass m, such that

$$\xi \in C(\mathbb{R}^+) \ , \ \xi(0) = 0, \ \ \forall m_1, m_2 > 0$$

$$\Longrightarrow \xi(m_1) + \xi(m_2) < \xi(m_1 + m_2) \ .$$

Note that it is satisfied by any convex function on $\mathbb{R}^+$ for which

$\xi(0) = 0$. For example:

$$\xi(m) = -m^\sigma \text{ if } 0 < \sigma < 1 \text{ , or } \xi(m) = m^\sigma \text{ if } \sigma > 1 \text{ .}$$

The dynamics of this system is obtained by the action: $A : \Gamma \to \mathbb{R}$ defined for $\gamma := (x_1, m_1 \dots x_N, m_M)$ by

$$A(\gamma; T) := \sum_1^N \int_0^T \left[\frac{1}{2} m_i(t) \left| \dot{x}_i \right|^2 - \xi(m_i(t)) \right] dt$$

Theorem If γ is a minimizer of the action A within the set Γ subjected to the end conditions $\gamma(0) = \left(x_1^{(0)}, m_1^{(0)} \dots x_N^{(0)}, m_N^{(0)} \right)$, $\gamma(T) = \left(x_1^{(T)}, m_1^{(T)} \dots x_N^{(T)}, m_N^{(T)} \right)$, then γ preserves both the linear momentum

$$\mathbf{P} := \sum_1^N m_i(t) \dot{x}_i(t)$$

and energy

$$\mathbf{E} := \frac{1}{2} \sum_1^N m_i(t) \left| \dot{x}_i(t) \right|^2 + \sum_1^N \xi(m_i(t)) \text{ .}$$

Implementation of the Inner energy

We now wish to extend the action principle to orbits composed of (Borel) measures in Ω. Let $\overline{\mathcal{M}}$ be the set of such probability Borel measures. For any $\mu \in \overline{\mathcal{M}}$ set $\mu = \mu^{pp} + \tilde{\mu}$ to be its *unique* decomposition into its atomic and non-atomic parts. For each $\mu \in \overline{\mathcal{M}}$ we define the inner energy $\Xi(\mu)$ as

$$\Xi(\mu) := \Xi(\mu^{pp}) = \sum_{x;\mu(\{x\})>0} \xi\left(\mu(\{x\})\right) \ .$$

For any $\mu \in \mathbf{H}_2([0,T])$ define the action as:

$$A_\Xi(\mu;T) := \frac{1}{2}\|\mu\|^2_{2,T} - \int_0^T \Xi(\mu_{(t)})dt \ .$$

We now pose the following assumptions on ξ:

$$\xi : \mathbb{R}^+ \to \mathbb{R}^+ \ , \quad \lim_{m\to 0} \frac{\xi(m)}{m} = 0 \qquad (**)$$

Remark: The assumption $\xi(m) = m^\sigma$ for $\sigma > 1$ verifies $(**)$.

Lemma: Suppose the inner energy function ξ satisfies $(**)$ Then the action $A_\Xi(\cdot, T)$ is lower-semi-continues (l.s.c) with respect to

$C\left([0,T]; C^*(\Omega)\right)$.

Theorem: Given $\mu_0, \mu_1 \in \overline{\mathcal{M}}$, there exists an action minimizer

$\mu \in \mathbf{H}_2[0,T]$ for

$$\underline{A}(\mu_0, \mu_1; T) := \min_\mu A_\Xi(\mu, T)$$

subjected to $\mu_{(0)} = \mu_0 \quad , \quad \mu_{(T)} = \mu_1$.

Remark: We cannot expect a *unique* minimizer. Even though $\|\cdot\|_2$ is a convex function on $\mathbf{H}_2$, the functional $-\int_0^T \Xi\left(\mu_{(t)}\right) dt$ is not convex!

What is the Euler Lagrange equation associated with the action A_Ξ ?

Relaxation:

We first consider a relaxation of the inner energy functional as follows: **Definition**: Let $J : \mathbb{R}^+ \to \mathbb{R}^+$ be a convex function satisfying $J(0) = J^{'}(0) = 0$. Let $\theta \in C_0^\infty(\Omega; \mathbb{R}^+)$ such that $\theta(0) = 1 \geq \theta(x)$ for all $x \in \Omega$. For each $\varepsilon > 0$, the inner energy function ξ corresponding to J is defined by

$$\xi(m) := \int_\Omega J(m\theta(x))dx \quad ; \quad m \geq 0 \; .$$

Let $\theta_\varepsilon(x) := \theta(x/\varepsilon)$ and

$$\Xi_\varepsilon(\mu) := \varepsilon^{-1} \int_\Omega J\left(\int_\Omega \theta_\varepsilon(x-y)\mu(dx)\right) dy \; .$$

The following is evident:

Lemma: For each $\varepsilon > 0$, $\mu \to -\int_0^T \Xi_\varepsilon\left(\mu_{(t)}\right) dt$ is continuous in the weak topology of $\mathbf{H}_2[0,T]$.

Let now

$$A_{\Xi}^{\varepsilon}(\mu;T) = \frac{1}{2}\|\mu\|_{2,T}^{2} - \int_0^T \Xi_\varepsilon\left(\mu_{(t)}\right) dt \ .$$

Theorem Given $\mu_0, \mu_1 \in \overline{\mathcal{M}}$, there exists an action minimizer for

$$\underline{A}_{\Xi}^{\varepsilon}(\mu_0, \mu_1; T) := \min_{\mu} A_{\Xi}^{\varepsilon}(\mu; T) \ .$$

Let μ_ε a minimizer of A_{Ξ}^{ε}. Since the set μ_ε, $0 < \varepsilon < 1$, is pre-compact in $\mathbf{H}_2[0,T]$, we can look for a limit point of a subsequence of μ_ε as $\varepsilon \to 0$.

Consider now the pair of equations

$$\frac{\partial \overline{\mu}}{\partial t} + \nabla \cdot (\overline{\mu} \nabla_x \psi) = 0$$

$$\frac{\partial \psi}{\partial t} + \frac{1}{2} |\nabla_x \psi|^2 - P_\varepsilon = 0 \ ,$$

where

$$P_\varepsilon = -\Xi_\varepsilon^{'}(\overline{\mu}_{(t)})_{(x,t)} := \varepsilon^{-1} \int_\Omega J^{'} \left(\int_\Omega \theta_\varepsilon(z-y) \overline{\mu}_{(t)}(dz) \right) \theta_\varepsilon(x-y) dy \ . \tag{1}$$

Theorem: If $\overline{\mu}^{(\varepsilon)}$ is a maximizer of the action $A^{\varepsilon}_{\underline{\Xi}}$ then there exists a reversible-pair solution $(\overline{\phi}^{(\varepsilon)}, \underline{\phi})^{(\varepsilon)}$ where P_ε given by (1). The reversibility set $K_0(\overline{\phi}^{(\varepsilon)}, \underline{\phi}^{(\varepsilon)})$ contains the support of $\overline{\mu}^{(\varepsilon)}$ in $\Omega \times (0, T)$. In addition, the reversibility set is invariant under the flow generated by the reversible solution

$$\frac{d\mathbf{T}_{(\varepsilon)}{}^{(s,t)}(x)}{dt} = \nabla \psi^{(\varepsilon)} \left(\mathbf{T}^{(s,t)}_{(\varepsilon)}(x), t \right) \ . \qquad (***)$$

As $\varepsilon \to 0$, the particles' orbits $\mathbf{T}^{(s,t)}_{(\varepsilon)}$ converge to a set-valued mapping $\mathbf{T}^{(s,t)} : \Omega \to \mathcal{B}(\Omega)$ so that $\lim_{\varepsilon \to 0} \mathbf{T}^{(s,t)}_{(\varepsilon)}(x) \in \mathbf{T}^{(s,t)}(x)$.

Suppose now an optimal transport is presented by the pair μ, ϕ where

$$\mu_{(t)}(dx) = \rho(x,t)dx + \sum m_i(t)\delta_{x_i(t)}dx \ ,$$

$$\int_\Omega \rho(x,t)dx + \sum m_i(t) = 1 \ . \quad (2)$$

where $x_i(t)$ are smooth trajectories and $m_i(t) > 0$ are smooth for $t \in [0,T]$.

The continuity equation takes the form

$$\frac{\partial \rho}{\partial t} + \nabla_x \cdot (\rho \nabla_x \psi) + \sum \dot{m}_i(t)\delta_{x_i(t)} = 0 \ .$$

and the momentum equation

$$\frac{\partial \psi}{\partial t} + \frac{1}{2}|\nabla_x \psi|^2 + \sum \xi^{'}\left(m_i(t)\right) \mathbf{1}(x_i(t) - x) = 0 \ ,$$

where $\mathbf{1}(x) = 0$ if $x \neq 0$, $\mathbf{1}(1) = 1$.

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Reversible solution in the limit $\varepsilon = 0$

The limit action function

$$C(y,x,\tau,t;\mu) := \inf_{\overline{x}} \left\{ \int_\tau^t \left(\frac{1}{2}|\dot{\overline{x}}(s)|^2 - \sum_{\mu_{(s)}(\{x\})>0} \xi^{'}(\mu_{(s)}(\{x\}))1_{(\overline{x}(s),s)} \right) ds \right\}$$

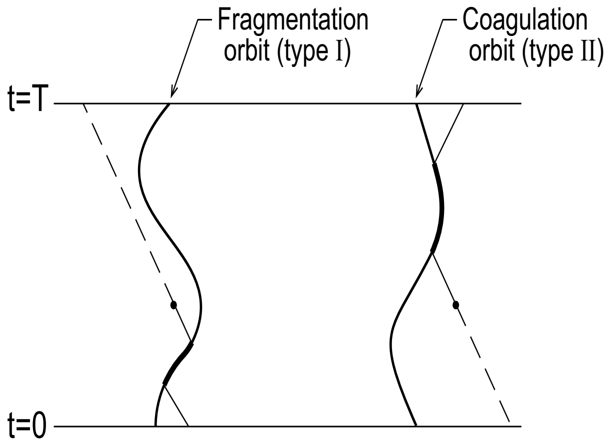
where the infimum is taken on the set of orbits $\overline{x} : [\tau, t] \to \Omega$ satisfying $\overline{x}(\tau) = y$, $\overline{x}(t) = x$.

Fragmentation:

$$\psi(x,t) = \inf_{y\in\Omega} [C(y,x,0,t;\mu) + \phi_0(y)] \le \overline{\phi}(x,t) := \inf_{y\in\Omega} \left[\frac{|x-y|^2}{2t} + \phi_0(y) \right] \tag{3}$$

Coagulation:

$$\underline{\phi}(x,t) := \sup_{y\in\Omega} \left[-\frac{|x-y|^2}{2(T-t)} + \phi_1(y) \right] \le \sup_{y\in\Omega} [C(x,y,t,T;\mu) + \phi_1(y)] = \psi(x,t) \tag{4}$$



A representation of a reversible solution. Bold curves: particle orbits. Bold dots: observers positions at time t. Light curves: the characteristic curves for forward (res. backward) solution in the vicinity of type (I) (res. type (II)) orbit. Dashed light lines: the characteristic curves for forward (res. backward) solution in the vicinity of type (II) (res. type (I)) orbit.

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. Representation of the solution:

$$\psi(x,t) = \psi_0(x,t) + \sum_i \alpha_i |x - x_i(t)| \quad , \quad \psi_0 \in C^1 \ .$$

$$\overline{\rho}_i(t) := \frac{1}{2}\left[\rho(x_i^-(t),t) + \rho(x_i^-(t),t)\right] \ .$$

Then

$$\frac{|\alpha_i|^2(t)}{8} - \xi^{'}(m_i(t)) = 0 \ ,$$

and

$$\text{Coagulation :} \quad \frac{dm_i}{dt} = \overline{\rho}_i(t)\sqrt{8\xi_i'(m_i)} \ .$$

$$\text{Fragmentation :} \quad \frac{dm_i}{dt} = -\overline{\rho}_i(t)\sqrt{8\xi_i'(m_i)} \ , \ .$$

while the particle's orbit satisfies the Rankine-Hugoniot condition:

$$\dot{x}_i = \frac{1}{2}\left[\psi_x(x_i^+(t),t) + \psi_x(x_i^-(t),t)\right]$$
$$:= \frac{\partial}{\partial x}\psi_0(x_i(t),t) + \sum_{j\neq i}\alpha_j(t)\frac{x_i(t) - x_j(t)}{|x_i(t) - x_j(t)|} \ . \quad (5)$$