Evolution PDEs under density constraints

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1. Micro and macro models for crowd motions with constraints
   - Disks with no overlapping
   - Density $\rho \leq 1$
   - Continuity equation, nonlinear diffusion, Hele-Shaw
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Modeling

Micro and macro models with constraints

Non-overlapping disks

A particle population moves, and each particle - if alone - would follow its own velocity u (depending on time, position... a typical case is : $u = -\nabla V$, where $V(x) = \text{dist}(x, \Gamma)$, Γ being an exit).

Yet, particles are (modeled by) rigid disks that cannot overlap, hence, the actual velocity v will not be u if u is too concentrating.

If q is the particle configuration, we define $adm(q)$ the set of velocities that do not induce overlapping : if every particle is a disk with radius R, located at q_i, we have

$$q \in K := \{q = (q_i)_i \in \Omega^N \ : \ |q_i - q_j| \geq 2R\}$$

$$adm(q) = \left\{v = (v_i)_i \ : \ (v_i - v_j) \cdot (q_i - q_j) \geq 0 \ \forall (i,j) \ : \ |q_i - q_j| = 2R\right\}$$

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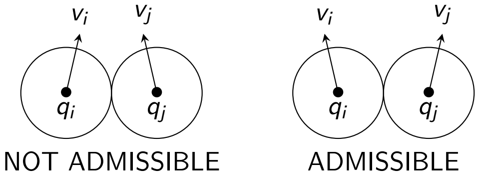


A general model

How to handle $v \approx u$ and $q \in K$ at the same time ?

We will assume $v = P_{adm(q)}[u]$ and solve $q'(t) = P_{adm(q(t))}[u_t]$ (with $q(0)$ given). This can be discretized (*catching-up algorithm*) as follows

$$\tilde{q}^{\tau}_{n+1} = q^{\tau}_n + \tau u_{n\tau}, \quad q^{\tau}_{n+1} = P_K[\tilde{q}^{\tau}_{n+1}]$$

(for a small time step $\tau > 0$) and is the same as the differential inclusion

$$q'(t) \in u_t - N_K(q(t))$$

where N_K is the normal cone to the set K

$$N_K(q_0) = \{v \,:\, q_1 \in K \Rightarrow v \cdot (q_1 - q_0) \leq o(|q_1 - q_0|)\}.$$

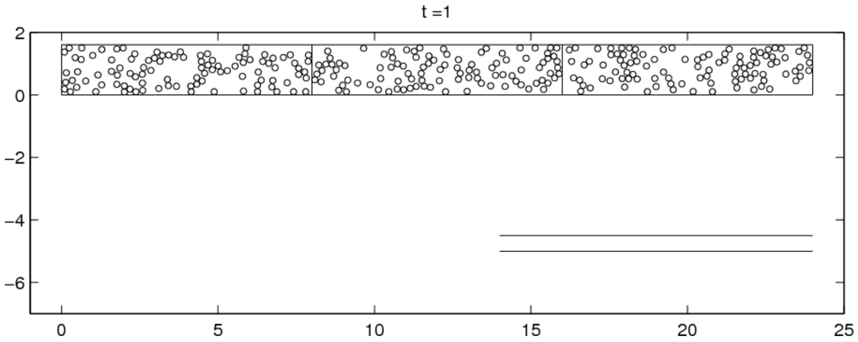
We exactly have a perturbed sweeping process with exterior forcing u.

It is important here that K, even if not convex in Ω^N, is as at least *prox-regular* (the projection on K is well defined on a neighborhood of K).

B. Maury, J. Venel, Handling of contacts in crowd motion simulations, *Traffic and Granular Flow '07*, 2009 ; A discrete contact model for crowd motion *ESAIM : M2AN*, 2011.

Commuters from the RER to the escalator

(numerical simulation by J. Venel)



Continuous formulation

- The particles population will be described by a density $\rho \in \mathcal{P}(\Omega)$,
- the constraint by $K = \{\rho \in \mathcal{P}(\Omega) \, : \, \rho \leq 1\}$,
- $u : \Omega \to \mathbb{R}^d$ will be a vector field, possibly depending on time or ρ,
- $adm(\rho) = \{v : \Omega \to \mathbb{R}^d \, : \, \nabla \cdot v \geq 0 \text{ on } \{\rho = 1\}\}$,
- P is the projection in $L^2(dx)$ or (which is the same) in $L^2(\rho)$,
- we'll solve $\partial_t \rho_t + \nabla \cdot \left(\rho_t \left(P_{adm(\rho_t)} u_t\right)\right) = 0$.

The equation $\partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0$ (*continuity equation*) is exactly the equation satisfied by the evolution of a density ρ when each particle follows the velocity field v (with $v \cdot n = 0$ on $\partial\Omega$, so that the density does not exit Ω).

Difficulty : $v = P_{adm(\rho_t)} u_t$ is not regular, neither depends regularly on ρ.

Pressures and duality

The set $adm(\rho)$ may be better described by duality :

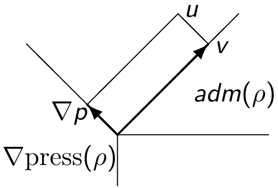
$$adm(\rho) = \left\{ v \in L^2(\rho) \ : \ \int v \cdot \nabla p \leq 0 \quad \forall p \ : \ p \geq 0, \ p(1-\rho) = 0 \right\}.$$

We can characterize $v = P_{adm(\rho)}(u)$ through

$$u = v + \nabla p, \quad v \in adm(\rho), \quad \int v \cdot \nabla p = 0,$$

$$p \in \mathrm{press}(\rho) := \{p \in H^1(\Omega), \ p \geq 0, \ p(1-\rho) = 0\}$$

This function p plays the role of a pressure affecting the movement.



$$\partial_t \rho_t + \nabla \cdot \big(\rho_t(u_t - \nabla p_t)\big) = 0$$

$$\rho_t \in K, \ p_t \in \mathrm{press}(\rho_t)$$

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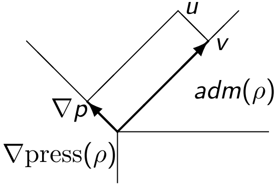


$$\color{red}{\partial_t \rho_t + \nabla \cdot (\rho_t u_t) - \Delta p_t = 0}$$

$$\rho_t \in K, \ p_t \in \mathrm{press}(\rho_t)$$

. . . very similar to the Hele-Shaw flow

The Hele-Shaw flow in few words :

$$\partial_t \rho_t - \Delta p_t = G_t \text{ (= reaction terms)}$$

where $p_t \in H(\rho_t)$ and H is a monotone graph. When $H(s) = s^m$ we have a **porous-medium equation** (non-linear diffusion), when $H = \partial I_{[0,1]}$ (hence $H(s) = [0, +\infty[$ for $s = 1$, $H(s) = \{0\}$ for $0 < s < 1$), the pressure $p \geq 0$ is arbitrary, but satisfies $p(1 - \rho) = 0$. (density dynamics)
When $G \geq 0$ and $\rho_0 = \mathbb{1}_{\Omega_0}$ is a patch, the evolution is $\rho_t = \mathbb{1}_{\Omega_t}$ with Ω_t evolving with normal velocity (free boundary geometric evolution)

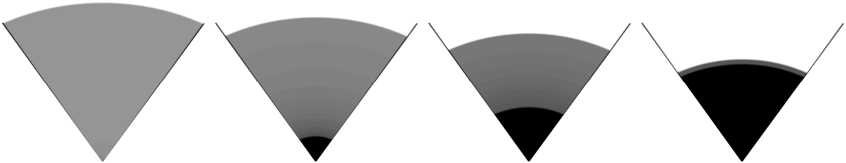
$$v_t = -\partial p_t / \partial n, \quad -\Delta p_t = G \text{ in } \Omega_t,\ p_t = 0 \text{ on } \partial\Omega_t.$$

Our PDE has the same form, with an advection term instead of reaction.

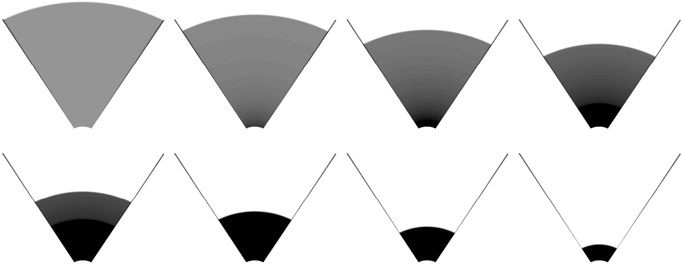
M.G. Crandall, An introduction to evolution governed by accretive operators, 1976
Ph. Bénilan, L. Boccardo, M. Herrero, On the limit of solution of $u_t = \Delta u^m$ as $m \to \infty$, 1989
B. Perthame, F. Quirós, J.-L. Vázquez, The Hele-Shaw Asymptotics for Mechanical Models of Tumor Growth, *ARMA*, 2014.

An example

Closed door (no-flux boundary conditions on $\partial\Omega$)



Open door (free flux on the bottom, i.e. mixed Dirichlet-Neumann for p)



Existence and approximation

The role of optimal transport

A splitting (catching-up) scheme for the PDE

Fix a time step $\tau > 0$. We look for a sequence $(\rho_n^\tau)_n$ where ρ_n^τ stands for ρ at time $n\tau$. We first define

$$\tilde\rho_{n+1}^\tau = (id + \tau u_{n\tau})_\# \rho_n^\tau \; ; \quad \rho_{n+1}^\tau = P_K(\tilde\rho_{n+1}^\tau)$$

where the projection P_K is in the sense of the Wasserstein distance, induced by optimal transport.

The key point is actually using the W_2 projection (instead of L^2 or other projections). It corresponds to the L^2 projection of velocity fields and of (Lagrangian) positions.

B. Maury, A. Roudneff-Chupin and F. Santambrogio, A macroscopic crowd motion model of gradient flow type, *Math. Mod. Meth. Appl. Sci.*, 2010

B. Maury, A. Roudneff-Chupin, F. Santambrogio and J. Venel, Handling congestion in crowd motion modeling *Net. Het. Media*, 2011

Optimal transport and Wasserstein distances

If two probabilities $\mu, \nu \in \mathcal{P}(\Omega)$ are given on a compact domain, the Monge-Kantorovich problem reads

$$\begin{aligned}\frac{1}{2}W_2^2(\mu,\nu) &= \inf\left\{\int \frac{1}{2}|x-T(x)|^2 d\mu \;:\; T:\Omega\to\Omega,\; T_\#\mu=\nu\right\}\\ &= \inf\left\{\int \frac{1}{2}|x-y|^2 d\gamma \;:\; \gamma\in\mathcal{P}(\Omega^2),\,(\pi_x)_\#\gamma=\mu,(\pi_y)_\#\gamma=\nu\right\}\\ &= \sup\left\{\int \phi\, d\mu+\int\psi\, d\nu \;:\; \phi(x)+\psi(y)\le\frac{1}{2}|x-y|^2\right\}.\end{aligned}$$

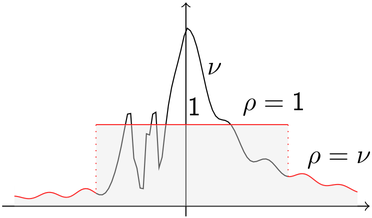
Under suitable assumptions, there exist an optimal transport T and an optimal ϕ, called **Kantorovich potential,** which is Lipschitz continuous. They are linked by $T(x) = x - \nabla\phi(x)$ (also, $T = \nabla u$ with $u(x) = |x|^2/2 - \phi(x)$ convex). Moreover, $W_2(\mu,\nu)$ is a distance on $\mathcal{P}(\Omega)$ which metrizes the weak-* convergence of probabilities (on compact domains).

G. Monge, Mémoire sur la théorie des déblais et des remblais, 1781
L. Kantorovich, On the transfer of masses, *Dokl. Acad. Nauk. USSR*, 1942.
Y. Brenier, Décomposition polaire et réarrangement monotone des champs de vecteurs, *CRAS*, 1987.

Projections and pressures

Fix a measure $\nu \in \mathcal{P}(\Omega)$ and solve

$$\min\left\{\frac{1}{2}W_2^2(\rho,\nu)\ :\ \rho\in K\right\} \quad = \quad \min_{\rho\leq 1}\ \sup_{\phi,\psi}\int\phi\,d\rho+\int\psi\,d\nu.$$



By duality and inf-sup exchange, the optimal ρ must also solve

$$\min\int\phi\,d\rho\ :\ \rho\leq 1,$$

where ϕ is the Kantorovich potential in the transport from ρ to ν. This implies

$$\exists\ell\ :\ \rho=\begin{cases}1 & \text{on } \phi<\ell,\\ 0 & \text{on } \phi>\ell,\\ \in[0,1] & \text{on } \phi=\ell\end{cases} \Rightarrow p:=(\ell-\phi)_+\geq 0,\ \ p(1-\rho)=0.$$

Hence, $p\in\mathrm{press}(\rho)$ and, passing to gradients, we have

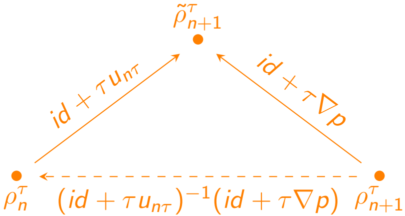
$$\rho-\text{a.e.}\quad \nabla p=-\nabla\phi=T(x)-x.$$

Getting back to the PDE

$T(x) = x + \nabla p(x)$ is the optimal transport from ρ^τ_{n+1} to $\tilde\rho^\tau_{n+1}$. Notice

$$||\nabla p||_{L^2(\rho^\tau_{n+1})} = W_2(\rho^\tau_{n+1}, \tilde\rho^\tau_{n+1}) \leq W_2(\rho^\tau_n, \tilde\rho^\tau_{n+1}) \leq \tau ||u_{n\tau}||_{L^2(\rho^\tau_n)}.$$

This suggest to scale the pressure (we call it now τp) and get the following situation



Formally, we have $(id + \tau u_{n\tau})^{-1}(id + \tau\nabla p) = id - \tau(u_{(n+1)\tau} - \nabla p) + o(\tau)$ provided u is regular enough. This allows to get, in the limit $\tau \to 0$, the vector field $v_t = P_{adm(\rho_t)}[u_t]$ and get a solution of the PDE.

Diffusive variants, different splitting methods

Add diffusion to the equation

$$\partial_t \rho_t + \nabla \cdot (\rho_t u_t) - \sigma \Delta \rho_t - \Delta p_t = 0$$

where $\sigma \geq 0$ is a volatility. We can't take anymore $\tilde{\rho}^\tau_{n+1} = (id + \tau u_{n\tau})_\# \rho^\tau_n$, but we can take the solution of the Fokker-Planck equation

$$\begin{cases} \partial_s \rho_s + \nabla \cdot (\rho_s u_s) - \sigma \Delta \rho_s = 0, \\ \rho_0 = \rho^\tau_n; \end{cases}$$

then, define $\tilde{\rho}^\tau_{n+1} = \rho_\tau$.

This gives a theoretically more efficient splitting scheme also for $\sigma = 0$. The method works and converges under the same assumptions for the FP equation to be well-posed : $u \in L^\infty$ if $\sigma > 0$, u satisfying DiPerna-Lions (or Ambrosio) theory for $\sigma = 0$ ($u \in W^{1,1}$ or $u \in BV$ + bounds on $\nabla \cdot u$).

R. J. DiPerna, P. L. Lions, Ordinary differential equations, transport theory and Sobolev spaces, *Inv. Math.*, 1989
L. Ambrosio Transport equation and Cauchy problem for BV vector fields, *Inv. Math.* 2003
A. R. Mészáros, F. Santambrogio Advection-diffusion equations with density constraints, *An. PDEs*, 2016.

The projection operator

A key tool is the projection operator $P_K[\nu] := \text{argmin}\{W_2^2(\rho,\nu), \rho \leq 1\}$. Its properties are essential for proving convergence. What we know :

- $W_2^2(\cdot,\nu)$ is strictly convex as soon as $\nu \ll \mathcal{L}^d$. This provides uniqueness and hence continuity in this case.
- Uniqueness actually holds for every ν, in the case $f \ll \mathcal{L}^d$.
- The geodesic convexity of $\{\rho : \rho \leq 1\}$ (w.r.t. Wasserstein geodesics) also gives uniqueness, and Hölder continuity w.r.t. W_2.
- (1-)Lipschitz continuity of P_K is an open question !
- The projection preserves ordering and decreases the L^1 distance between densities.
- Estimates (order 0) : for every convex U, $\rho \mapsto \int U(\rho(x))dx$ decreases under projection.
- Estimates (order 1) : the BV norm decreases under projection.

A. Roudneff-Chupin, Modélisation macroscopique de mouvements de foule, PhD thesis, Orsay, 2011
G. De Philippis, A. R. Mészáros, F. Santambrogio, B. Velichkov BV estimates in optimal transportation and applications, *ARMA*, 2016.

Evolving domains and measure sweeping processes

What if the domain Ω is a convex set $\Omega(t)$ evolving in time ?

$$\begin{cases} \partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0 & \text{in } \Omega(t), \\ v_t(x) \in -N_{\Omega(t)}(x), \\ \text{spt}(\rho_t) \subset \Omega(t). \end{cases}$$

Unconstrained

$$\begin{cases} \partial_t \rho_t - \Delta p_t = 0 & \text{in } \Omega(t), \\ p_t \geq 0, \rho_t \leq 1, p_t(1-\rho_t) = 0 & \text{in } \Omega(t) \\ \text{spt}(\rho_t) \subset \Omega(t). \end{cases}$$

Density constraints

It is enough to project in the space $W_2(\mathbb{R}^d)$ onto $K = \{\rho \in \mathcal{P}(\mathbb{R}^d) : \text{spt}(\rho) \in \Omega(t)\}$ or $K = \{\rho \in \mathcal{P}(\mathbb{R}^d) : \text{spt}(\rho) \in \Omega(t), \rho \leq 1\}$.

$$\begin{cases} \partial_t \rho_t - \sigma \Delta \rho_t = 0 & \text{in } \Omega(t), \\ -\sigma \nabla \rho_t \cdot n = \rho_t V_t & \text{on } \partial\Omega(t), \\ \text{spt}(\rho_t) \subset \Omega(t). \end{cases}$$

Diffusion

$$\begin{cases} \partial_t \rho_t - \sigma \Delta \rho_t - \Delta p_t = 0, \\ p_t \geq 0, \rho_t \leq 1, p_t(1-\rho_t) = 0 & \text{in } \Omega(t) \\ \text{spt}(\rho_t) \subset \Omega(t). \end{cases}$$

Diffusion + constraints

S. Di Marino, B. Maury, F. Santambrogio Measure sweeping processes, *J. Conv. An.*, 2016. Constraints / Small Diffusion / Larger Diffusion / Diffusion+constraints

Gradient flows

When u has a suitable gradient structure, it is possible to do the two steps of the splitting algorithm at once, thanks to the theory of gradient flows.
Gradient flows in few words : consider an evolution equation of the kind

$$x'(t) = -\nabla F(x(t))$$

(we follow the steepest descent lines of a function $F : \mathbb{R}^n \to \mathbb{R}$). We can discretize in time such an equation by solving

$$x^\tau_{k+1} \in \text{argmin}_x \, F(x) + \frac{1}{2\tau}|x - x^\tau_k|^2, \quad \tau > 0 \text{ fixed.}$$

The optimal x^τ_{k+1} satisfies

$$\frac{x^\tau_{k+1} - x^\tau_k}{\tau} + \nabla F(x^\tau_{k+1}) = 0$$

which corresponds to an implicit Euler scheme for $x' = -\nabla F(x)$, the solution being found as a limit $\tau \to 0$.
This formulation may easily be adapted to a general metric space...

E. De Giorgi, New problems on minimizing movements, *Boundary Value Problems for PDE and Applications*, 1993

Gradient flows in W_2

Let F be a functional over $(\mathcal{P}(\Omega), W_2)$, and let us follow the so-called JKO scheme

$$\rho^\tau_{k+1} \in \operatorname{argmin}_\rho F(\rho) + \frac{W_2^2(\rho, \rho^\tau_k)}{2\tau}$$

Discrete optimality conditions :

$$\frac{\delta F}{\delta \rho}(\rho^\tau_{k+1}) + \frac{\phi}{\tau} = const$$

which implies

$$v(x) := \frac{x - T(x)}{\tau} = \frac{\nabla \phi(x)}{\tau} = -\nabla\Big(\frac{\delta F}{\delta \rho}(\rho)\Big)$$

and, since v represents the discrete velocity (displacement / time step), at the limit $\tau \to 0$ the continuity equation $\partial_t \rho + \nabla \cdot (\rho v) = 0$ gives

$$\partial_t \rho - \nabla \cdot \Big(\rho \nabla\Big(\frac{\delta F}{\delta \rho}(\rho)\Big)\Big) = 0.$$

R. Jordan, D. Kinderlehrer, F. Otto, The variational formulation of the Fokker-Planck equation, *SIAM J. Math. Anal.*, 1998.

Examples

Take $F(\rho) = \int U(\rho(x))dx$. Then $\frac{\delta F}{\delta \rho}(\rho) = U'(\rho)$. The equation becomes

$$\partial_t \rho - \nabla \cdot \big(\rho \nabla U'(\rho)\big) = 0.$$

For instance, for $U(t) = t \log t$ we get $\nabla U'(\rho) = \frac{\nabla \rho}{\rho}$, which gives the heat equation $\partial_t \rho - \Delta \rho = 0$. For $F(\rho) = \int V(x) d\rho$ we get $\frac{\delta F}{\delta \rho}(\rho) = V$, and we obtain the Fokker-Planck equation with $F(\rho) = \int V(x)d\rho + \int \rho \log \rho \ldots$

The equation $\partial_t \rho - \nabla \cdot (\rho \nabla V) - \Delta p = 0$ (with $p(1-\rho) = 0$) is the gradient flow of the functional

$$F(\rho) = \begin{cases} \int V(x) d\rho & \text{if } \rho \in K, \\ +\infty & \text{if not,} \end{cases}$$

which is the limit as $m \to \infty$ of the functional $\int (\frac{1}{m}\rho(x)^m + V(x)\rho(x))dx$. For the diffusive variant, just add $\sigma \int \rho(x) \log \rho(x) dx$; for diffusion on $\Omega(t)$, add this entropy and optimize among measures supported in $\Omega(t)$.

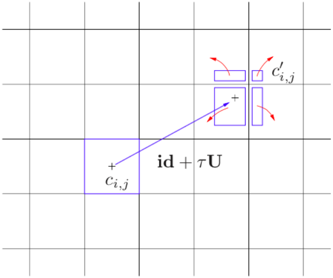
L. Ambrosio, N. Gigli, G. Savaré *Gradient Flows*, Birkäuser, 2005
F. Santambrogio {Euclidean, Metric, and Wasserstein} Gradient Flows : an overview, *Bull. Math. Sci.*, 2017.

Numerics

Optimal transport methods
for JKO or splitting schemes

Optimization of transport costs

In a splitting method, we first have to compute $(id + \tau u)_{\#}\rho_n$ (or to solve a PDE without density constraints), then to compute a projection, i.e. minimize a transport cost with a constraint on the final density ; in the JKO scheme, we directly minimize with a constraint and a penalization on the final density.



Yet, given ν, how to solve

$$\min\{W_2^2(\rho,\nu),\ \rho \leq 1\}$$

or, more generally

$$\min\{W_2^2(\rho,\nu) + F(\rho)\} \quad ?$$

Optimization methods for JKO - Augmented Lagrangian

Use the so-called Benamou-Brenier formula

$$W_2^2(\nu,\mu) = \min \left\{ \int\int \rho|v|^2 \,:\, \partial_t\rho + \nabla\cdot(\rho v) = 0, \rho_0 = \nu, \rho_1 = \mu \right\}.$$

Write $E = \rho v$, so that $\rho|v|^2 = |E|^2/\rho$ which is convex in (ρ, E). The minimization can be written (by duality) as a saddle point for a Lagrangian

$$L(m,(A,\phi)) := m\cdot(A - \nabla_{t,x}\phi) - K^*(A) + G(\phi),$$

where $m := (\rho, E)$, A is the dual variable to m, and $\nabla_{t,x}\phi := (\partial_t\phi, \nabla\phi)$ involves the test function for the constraint.

Augmented Lagrangian : use $\tilde{L}(m,(A,\phi)) := L(m,(A,\phi)) - \frac{r}{2}||A - \nabla_{t,x}\phi||^2$ (same saddle points as L, but more strictly convex). Saddle points can be approximated by alternate minimization.

When F is convex in μ, this can be adapted to solve $\min\{W_2^2(\rho,\nu) + F(\rho)\}$.

Example 1 — Example 2 — Example 3

J.-D. Benamou, Y. Brenier A computational fluid mechanics solution to the Monge-Kantorovich mass transfer problem, *Numer. Math.*, 2000.
J.-D. Benamou, G. Carlier, M. Laborde An augmented Lagrangian approach to Wasserstein gradient flows and applications, *ESAIM : Proc.*, 2016.

Optimization methods for JKO - discrete convex functions

We can rewrite the problem as

$$\min_{u \text{ convex } : \nabla u \in \Omega} \quad \frac{1}{2}\int_\Omega |\nabla u(x) - x|^2 d\nu + F((\nabla u)_\# \nu).$$

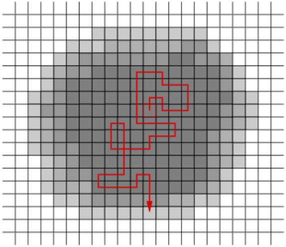
This problem is convex in u essentially when F is geodesically convex. Suppose that ν is discrete, $\nu = \sum_j a_j \delta_{x_j}$. A convex function defined on $\{x_j\}_j$ is a function $u : S \to \mathbb{R}$ such that for every $x \in S$ we have

$$\partial u(x) := \{p \in \mathbb{R}^d \ : \ u(x) + p \cdot (y - x) \leq u(y) \text{ for all } y \in S\} \neq \emptyset.$$

When F has the form $F(\rho) = \int U(\rho(x))dx$ we need to associate with $(\nabla u)_\# \nu$ a diffuse measure : let us spread the mass a_j uniformly on $\partial u(x_j)$. Then, it is possible to optimize, using a Newton algorithm, the functional by means of **computational geometry tools** which compute and differentiate the volumes of the subdifferential cells. The new measure ρ can be defined as $\rho = \sum_j a_j \delta_{y_j}$ where y_j is the barycenter of $\partial u(x_j)$. Example1 Example2

J.-D. Benamou, G. Carlier, Q. Mérigot and É. Oudet Discretization of functionals involving the Monge-Ampère operator, *Num. Math.*, 2016.

A stochastic approach to the projection operator



Remember that $\rho = P_K(\nu)$ means $\nu = (id + \nabla p)_{\#}\rho$, with $p \in \mathrm{press}(\rho)$, and $\rho = 1$ on $\{\rho \neq \nu\}$.
Hence, infinitesimally (i.e. when $(\nu - 1)_+$ is small), setting $A := \{\nu > 1\}$, we can find ρ just by letting A evolve into A' with normal velocity equal to $-\partial p/\partial n$ (with $-\Delta p = \nu - 1$ on A and $p = 0$ on ∂A) and setting $\rho = 1$ on A' and $\rho = \nu$ elsewhere.

A useful probabilistic fact : The law of the first exit point through ∂A of $(X + B_t)$, with $X \sim \mu$ on A and (B_t) is a Brownian motion independent of X, is the measure $(-\partial p/\partial n) \cdot \mathcal{H}^{d-1}_{|\partial A}$, where $-\Delta p = \mu$ on A and $p = 0$ on ∂A.

Algorithm : pick a random pixel among sorted according to $(\nu - 1)_+$ and start a random walk from there ; as soon as it meets a pixel with $\nu < 1$, leave there as much mass as you can and go on. Repeat till there is some excess. Use the obtained measure as ρ.

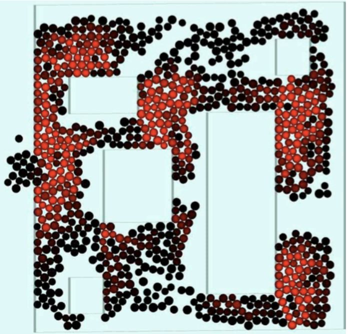
Warning : it works well in practice, but nothing is proven on the convergence of this approximation.

Micro vs Macro

5 obstacles, micro — 5 obstacles, macro

Micro vs Macro

5 obstacles, micro — 5 obstacles, macro



The End

Thanks for your attention