A new transportation distance with bulk/interface interactions and flux penalization: Models and Numerical aspects

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General Problem

Given two probabiblity measures $\mu, \nu \in \mathcal{P}(\Omega)$ and a cost function$c$ we want to solve the Monge problem as:

$$(MP) : \inf \int \{c(x, T(x)) d\mu(x) : T_{\sharp\mu} = \nu\} \tag{2}$$

where T is a transport plan.

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- Static Optimal Transport where we look for this maps which is a Lagragian point of view
- Dynamical Optimal Transport which is an Eulerian point of view.

Plan

Definition

Benamou-Brenier Formulation,00'

Let ρ_0, ρ_1, two probability measures:

$$W_2^2(\rho_0, \rho_1) = \begin{cases} \min\limits_{\rho, M} \int_0^1 \int_{\bar{\Omega}} \frac{||M||^2}{2\rho} dt \\ \partial_t \rho_t + \mathit{div} M = 0 \\ \rho(0) = \rho_0; \rho(1) = \rho_1 \end{cases} \tag{3}$$

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This problem is equivalent to finding a saddle point of the following augmented Lagrangian:

$$\begin{aligned} L_{rBB}(\varphi, q, \mu) = & \mathcal{F}_{BB}(\varphi) + \mathcal{G}_{BB}(q) + \iint_{Q_\Omega} (\partial_t \varphi - a) d\rho + \iint_{Q_\Omega} (\nabla \varphi - b) dM \\ & + \frac{r}{2} \iint_{Q_\Omega} |\partial_t \varphi - a|^2 + \frac{r}{2} \iint_{Q_\Omega} |\nabla \varphi - b|^2 \end{aligned} \tag{4}$$

where $q = (a, b)$ and $\mu = (\rho, M)$.

Where

$$\mathcal{F}_{BB}(\varphi) = \int_{\bar{\Omega}} \varphi(0,.)d\rho_0 - \int_{\bar{\Omega}} \varphi(1,.)d\rho_1 \qquad \mathcal{G}_{BB}(q) = \iint_{\bar{Q}} \iota_{S_\Omega}(a,b)dxdt \tag{5}$$

and ι_{S_Ω} is the convex analysis indicator over the set:

$$S_\Omega = \left\{ a \in \mathbb{R}, b \in \mathbb{R}^d, s.t : a + \frac{|b|^2}{2} \leqslant 0 \right\} \tag{6}$$

Algorithm BB

Algorithm 1 ALG2 BB

Given $(\varphi^{n-1}, q^{n-1}, \mu^{n-1})$

Step 1: Find φ^n such that:

$$\varphi^n = \arg\min_{\varphi} L_{rBB}(\varphi, q^{n-1}, \mu^{n-1}) \qquad \text{for fixed } (q^{n-1}, \mu^{n-1})$$

Step 2: Find q^n such that:

$$q^n = \arg\min_{q} L_{rBB}(\varphi^n, q, \mu^{n-1}) \qquad \text{for fixed } (\varphi^n, \mu^{n-1})$$

Step 3: Update μ using a gradient ascent step

$$\mu^n = \mu^{n-1} + r.(\partial_t \varphi^n - a^n, \nabla \varphi^n - b^n)$$

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Unbalanced Optimal transport: The Wasserstein Fisher-Rao metrics is defined by:

$$W_{FR}(\rho_0, \rho_1) = \min \left\{ \iint_{Q_\Omega} \frac{|G|^2}{2\rho} + \kappa^2 \iint_{Q_\Omega} \frac{|f|^2}{2\rho}, \qquad \text{s.t. : } \partial_t \rho + div\, G = f \right\} \tag{7}$$

Dynamical formulation of optimal transport

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This problem yields to solve a saddle point of the following Lagrangian:

$$
\begin{aligned}
L_{rWFr}(\varphi,q,\mu) =& \mathscr{F}_{WFr}(\varphi)+\mathscr{G}_{WFr}(q)+\iint_{Q_\Omega}(\partial_t\varphi-a)d\rho+\iint_{Q_\Omega}(\nabla\varphi-b)dG \\
&+\iint_{Q_\Omega}(\varphi-c).df+\frac{r}{2}\iint_{Q_\Omega}|\partial_t\varphi-a|^2 \\
&+\frac{r}{2}\iint_{Q_\Omega}|\nabla\varphi-b|^2+\frac{r}{2}\iint_{Q_\Omega}|\varphi-c|^2
\end{aligned}
$$

Where

$$
\mathscr{F}_{WFr}(\varphi,\psi)=\int_{\bar\Omega}\varphi(0,.)d\rho_0-\int_{\bar\Omega}\varphi(1,.)d\rho_1 \qquad \mathscr{G}_{WFr}(q)=\iint_{\bar\Omega}\iota_{S^\kappa_\Omega}(a,b,c)
$$

and $\iota_{S^\kappa_\Omega}$ is the convex analysis indicator over the set:

$$
S^\kappa_\Omega=\left\{(a,b,c),\mathbb{R}\times\mathbb{R}^{d-1}\times\mathbb{R}, \qquad \text{s.t. : } a+\frac{|b|^2}{2}+\frac{|c|^2}{2\kappa^2}\leqslant 0\right\}. \tag{8}
$$

Algorithm 2 ALG2 WFR

Given $(\varphi^{n-1}, q^{n-1}, \mu^{n-1})$

Step 1-a: Find φ^n such that

$$\varphi^n = \arg\min_{\varphi} L_{rWFr}(\varphi, q^{n-1}, \mu^{n-1}) \qquad \text{for fixed } (q^{n-1}, \mu^{n-1})$$

Step 2: Find q^n such that:

$$(q^n) = \arg\min_{q} L_{rWFr}(\varphi^n, q, \mu^{n-1}) \qquad \text{for fixed } (\varphi^n, \mu^{n-1})$$

Step 3: Update μ using a gradient ascent step

$$\mu^n = \mu^{n-1} + r.(\partial_t \varphi^n - a^n, \nabla \varphi^n - b^n, \varphi^n - c^n)$$

Plan

Model definition

In order to extend this model over a domain Ω of dimension d and his boundary Γ of dimension $d-1$ we need two continuity equations defined as follows:

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$$\begin{cases} \partial_t \omega + divF = 0 \text{ in } \Omega \\ F \cdot \nu = f \end{cases} \tag{9}$$

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- (9) is the classical continuity equation inside the domain , with F the momentum of the density ω. The particularity of the equation is the second line which means that the normal momentum outflux equals the variable f.
- (10) is the unbalanced optimal transport continuity equation where the source term f come from the inner domain.

This bi-formulation induced the following functional:

$$\iint_{Q_\Omega} \frac{|F|^2}{2\omega} + \iint_{Q_\Gamma} \frac{|G|^2}{2\gamma} + \kappa^2 \iint_{Q_\Gamma} \frac{|f|^2}{2\gamma} \tag{11}$$

Definition of W_κ

Let $\rho_0 = (\omega_0, \gamma_0), \rho_1 = (\omega_1, \gamma_1) \in \mathscr{P}^{\oplus}(\bar{\Omega})$, then the following minimization problem:

$$W_\kappa(\rho_0, \rho_1) = \min \iint_{Q_\Omega} \frac{|F|^2}{2\omega} + \iint_{Q_\Gamma} \frac{|G|^2}{2\gamma} + \kappa^2 \iint_{Q_\Gamma} \frac{|f|^2}{2\gamma} \tag{12}$$

$$s.t: \begin{cases} \partial_t \omega + divF = 0 \text{ in } \Omega \\ F.\nu = f \\ \partial_t \gamma + divG = f \text{ in } \Gamma \end{cases} \tag{13}$$

define a distance over the set $\mathscr{P}^{\oplus}(\bar{\Omega})$.

Plan

Properties of W_κ

Due to the non common definition of the distance W_κ it is interesting to check what happen to W_κ when the toll is varying. It has been shown that:

Theorem

For fixed $(\rho_0, \rho_1) \in \mathscr{P}^{\oplus}(\bar{\Omega})$ *one has that:*

1. $\lim\limits_{\kappa \longrightarrow \infty} W_\kappa(\rho_0, \rho_1) = W_{\bar{\Omega}}(\omega_0, \omega_1) + W_\Gamma(\gamma_0, \gamma_1)$
2. $\lim\limits_{\kappa \longrightarrow 0} W_\kappa(\rho_0, \rho_1) = W_{\bar{\Omega}}(\varrho_0, \varrho_1)$, *with* $\varrho_0 = \omega_0 + \gamma_0$ *and* $\varrho_1 = \omega_1 + \gamma_1$

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Continuity equations

Let φ and ψ be test functions mainly we take $\varphi \in \mathscr{C}^1(Q_\Omega)$ and $\psi \in \mathscr{C}^1(Q_\Gamma)$, the constraints are equivalent in weak sense to:

$$\iint_{Q_\Omega} \partial_t \varphi d\omega + \iint_{Q_\Omega} \nabla\varphi . dF - \iint_{Q_\Gamma} \varphi df = \int_\Omega \varphi(1,.) d\omega_1 - \int_\Omega \varphi(0,.) d\omega_0 \tag{14}$$

$$\iint_{Q_\Gamma} \partial_t \psi d\gamma + \iint_{Q_\Gamma} \nabla\psi . dG + \iint_{Q_\Gamma} \psi df = \int_\Gamma \psi(1,.) d\gamma_1 - \int_\Gamma \psi(0,.) d\gamma_0 \tag{15}$$

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$$\iint_{Q_\Gamma} \partial_t \psi d\gamma + \iint_{Q_\Gamma} \nabla\psi . dG + \iint_{Q_\Gamma} \psi df = \int_\Gamma \psi(1,.) d\gamma_1 - \int_\Gamma \psi(0,.) d\gamma_0 \quad (15)$$

So we can write the corresponding Lagrangian as follows:

$$\begin{aligned} L(\varphi,\psi,F,G,f,\omega,\gamma) = &\iint_{Q_\Omega} \frac{|F|^2}{2\omega} - \iint_{Q_\Omega} \partial_t \varphi d\omega - \iint_{Q_\Omega} \nabla\varphi\, dF + \iint_{Q_\Gamma} \varphi.df \\ &+ \int_\Omega \varphi(1,.)d\omega_1 - \int_\Omega \varphi(0,.)d\omega_0 \\ &+ \iint_{Q_\Gamma} \frac{|G|^2}{2\gamma} + \kappa^2 \iint_{Q_\Gamma} \frac{|f|^2}{2\gamma} - \iint_{Q_\Gamma} \partial_t\psi d\gamma \\ &- \iint_{Q_\Gamma} \nabla\psi.dG - \iint_{Q_\Gamma} \psi df + \int_\Gamma \psi(1,.)d\gamma_1 \\ &- \int_\Gamma \psi(0,.)d\gamma_0 \end{aligned} \tag{16}$$

We got a saddle point problem with $q = (\alpha, \beta, a, b, c)$ and $\mu = (\omega, F, \gamma, G, f)$.

$$
\begin{aligned}
-\inf_{\varphi,\psi,q} \sup_{\mu} L = \sup_{\mu} \inf_{\varphi,\psi,q} \Big\{ & \mathscr{F}(\varphi,\psi) + \mathscr{G}(q) + \iint_{Q_\Omega} (\partial_t \varphi - \alpha) d\omega \\
& + \iint_{Q_\Omega} (\nabla \varphi - \beta) dF + \iint_{Q_\Gamma} ({\color{red}\psi} - c - {\color{red}\varphi}).df + \\
& \iint_{Q_\Gamma} (\partial_t \psi - a) d\gamma + \iint_{Q_\Gamma} (\nabla \psi - b).dG \Big\}
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$$- \inf_{\varphi,\psi,q} \sup_{\mu} L = \sup_{\mu} \inf_{\varphi,\psi,q} \Big\{ \mathscr{F}(\varphi,\psi) + \mathscr{G}(q) + \iint_{Q_\Omega} (\partial_t \varphi - \alpha) d\omega + \iint_{Q_\Omega} (\nabla \varphi - \beta) dF + \iint_{Q_\Gamma} (\psi - c - \varphi).df + \iint_{Q_\Gamma} (\partial_t \psi - a) d\gamma + \iint_{Q_\Gamma} (\nabla \psi - b).dG \Big\} \tag{17}$$

- $\mathscr{G}$ is the convex indicator over the set $S_\Omega \times S_\Omega^\kappa$.
- no coercivity/linearity.
- augmented Lagrangian $\forall r > 0$

$$
\begin{aligned}
L_r = & \mathscr{F}(\varphi,\psi) + \mathscr{G}(q) + \iint_{Q_\Omega} (\partial_t\varphi - \alpha) d\omega + \iint_{Q_\Omega} (\nabla\varphi - \beta) dF + \iint_{Q_\Gamma} (\psi - c - \varphi).df \\
& + \iint_{Q_\Gamma} (\partial_t\psi - a) d\gamma + \iint_{Q_\Gamma} (\nabla\psi - b).dG + \frac{r}{2}\iint_{Q_\Omega} |\partial_t\varphi - \alpha|^2 \\
& + \frac{r}{2}\iint_{Q_\Omega} |\nabla\varphi - \beta|^2 + \frac{r}{2}\iint_{Q_\Gamma} |\nabla\psi - b|^2 \\
& + \frac{r}{2}\iint_{Q_\Gamma} |\psi - \varphi - c|^2 + \frac{r}{2}\iint_{Q_\Gamma} |\partial_t\psi - a|^2
\end{aligned}
$$

Algorithm 3 ALG2 W_κ

Given $(\varphi^{n-1}, \psi^{n-1}; q^{n-1}, \mu^{n-1})$

Step 1-a: Find φ^n such that

$$\varphi^n = \arg\min_{\varphi} L_r(\varphi, \psi^{n-1}, q^{n-1}, \mu^{n-1}) \qquad \text{for fixed } (\psi^{n-1}, q^{n-1}, \mu^{n-1})$$

Step 1-b: Find ψ^n such that

$$\psi^n = \arg\min_{\psi} L_r(\varphi^n, \psi, q^{n-1}, \mu^{n-1}) \qquad \text{for fixed } (\varphi^n, q^{n-1}, \mu^{n-1})$$

Step 2: Find q^n such that:

$$q^n = \arg\min_{q} L_r(\varphi^n, \psi^n, q, \mu^{n-1}) \qquad \text{for fixed } (\varphi^n, \psi^n, \mu^{n-1})$$

Step 3: Update μ using a gradient ascent step

$$\mu^n = \mu^{n-1} + r.(\partial_t\varphi^n - \alpha^n, \nabla\varphi^n - \beta^n, \partial_t\psi^n - a^n, \nabla\psi^n - b^n, \psi^n - c^n - \varphi)$$

Step 1a: We want to solve the minimization problem in φ. So we differentiate the augmented Lagrangian with respect to φ and get the following variation formula:

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$$\begin{cases} -\Delta_{t,x}\varphi^n = \dfrac{1}{r}div_{t,x}(\omega^{n-1}, F^{n-1}) - div_{t,x}(\alpha^{n-1}, \beta^{n-1}) \\ r\partial_\nu \varphi^n + \varphi^n = (r\beta^{n-1} - F^{n-1}).\nu + f^{n-1} + r(\psi^{n-1} - c^{n-1}) \\ r\partial_t \varphi^n(0,.) = \omega_0 - \omega^n(0,.) + r\alpha^{n-1}(0,.) \\ r\partial_t \varphi^n(1,.) = \omega_1 - \omega^n(1,.) + r\alpha^{n-1}(1,.) \end{cases} \tag{18}$$

The (18) is an elliptic PDE with Robin boundaries conditions in space and Neumann boundaries conditions in time.

Step 1b: The target is the same as in the previous one so we have on the boundary:

$$\begin{cases} -\Delta_{t,x}\psi^n + \psi = \dfrac{1}{r}\nabla_{t,x}(\gamma^{n-1}, G^{n-1}) - \nabla_{t,x}(a^{n-1}, b^{n-1}) - \dfrac{1}{r}f + c^{n-1} + \varphi^n \\ s.t \text{ boundaries conditions :} \\ r\partial_t\psi^n(0,.) = \gamma_0 - \gamma^n(0,.) + ra(0,.)^{n-1} \\ r\partial_t\psi^n(1,.) = \gamma_1 - \gamma^n(1,.) + ra(1,.)^{n-1} \end{cases} \tag{19}$$

This elliptic (19) have Neumann boundaries conditions in time and No boundary conditions in space due to the particular domain Γ.

Plan

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Conclusion

we apply a really classic tools to solve dynamical optimal tranport to the new distanceW_κ namely ALG2 W_κ and to make some simulations in 2D time space.

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Futur work

we tried to implement it on the circle in 2D and a cylinder in 3d time space but we got a divergence during the iterations; probably due to errors in numerical considerations.

- The first one could be to try to investigate and understand what kind of subtlety we lost during our 3d attempt.
- Illustrate numerically the large toll limit and the small toll
- Maybe try to solve it with the coupled sytems in (φ, ψ) simultaneously.
- Another avenue would be to question the augmented Lagrangian method for this problem, which is much more delicate than conventional and unbalanced transport: we could attempt a new numerical scheme .

Merci pour votre aimable attention!!

Properties of W_κ

Theorem

For fixed $(\rho_0, \rho_1) \in \mathscr{P}^{\oplus}(\bar{\Omega})$ *one has that:*

$$\lim_{\kappa \longrightarrow 0} W_\kappa(\rho_0, \rho_1) = W_{\bar{\Omega}}(\varrho_0, \varrho_1)$$

with $\varrho_0 = \omega_0 + \gamma_0$ *and* $\varrho_1 = \omega_1 + \gamma_1$

Sketch of the proof

We want to show that $\limsup W_\kappa^2(\rho_0, \rho_1) \leqslant W_{\bar\Omega}^2(\varrho_0, \varrho_1)$, where $\rho_0 = (\omega_0, \gamma_0)$, $\rho_1 = (\omega_1, \gamma_1)$, $\varrho_0 = \omega_0 + \gamma_0$ and $\varrho_1 = \omega_1 + \gamma_1$.
In order to achieve this goal we will connect $\rho_0 \rightsquigarrow \rho_0^\kappa = (\omega_0 + \gamma_0, 0)$ using a Fisher-Rao geodesic and then transport ρ_0^κ to $\rho_1^\kappa = (\omega_1 + \gamma_1, 0)$ using a classical Wasserstein geodesic and finally we will connect$\rho_1^\kappa \rightsquigarrow \rho_1$ using again a Fisher-Rao geodesic

- Connecting $\rho_0 \rightsquigarrow \rho_0^\kappa = (\omega_0 + \gamma_0, 0)$ using Fischer Rao metrics yields to:

$$W^2(\rho_0, \rho_0^\kappa) = 2\kappa^2 \int_\Gamma \gamma_0 \tag{20}$$

Sketch of the proof

We want to show that $\limsup W_\kappa^2(\rho_0,\rho_1) \leqslant W_\Omega^2(\varrho_0,\varrho_1)$, where $\rho_0 = (\omega_0,\gamma_0)$, $\rho_1 = (\omega_1,\gamma_1)$, $\varrho_0 = \omega_0 + \gamma_0$ and $\varrho_1 = \omega_1 + \gamma_1$.
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$$W^2(\rho_0,\rho_0^\kappa) = 2\kappa^2 \int_\Gamma \gamma_0 \tag{20}$$

- Let's compute the cost for transport from $\rho_0^\kappa = (\omega_0 + \gamma_0; 0)$ to $\rho_1^\kappa = (\omega_1 + \gamma_1; 0)$ We can use the fact that it's just classical transportation and we got that:

$$W_\kappa^2(\rho_0^\kappa;\rho_1^\kappa) = W_\Omega^2(\omega_0 + \gamma_0 + 0, \omega_1 + \gamma_1 + 0) = W_\Omega^2(\varrho_0,\varrho_1) \tag{21}$$

Sketch of the proof

- Connecting $\rho_1^\kappa \rightsquigarrow \rho_1$, we got that:

$$W^2(\rho_1, \rho_1^\kappa) = 2\kappa^2 \int_\Gamma \gamma_0 \tag{22}$$

Finally we have that:

$$\limsup W_\kappa^2(\rho_0, \rho_1) \leqslant \limsup 2\kappa^2 \int_\Gamma \gamma_0 + W_{\bar{\Omega}}^2(\varrho_0, \varrho_1) + \limsup 2\kappa^2 \int_\Gamma \gamma_1 = W_{\bar{\Omega}}^2(\varrho_0, \varrho_1) \tag{23}$$