NUMERICAL CONSIDERATIONS ON AN ISOPERIMETRIC PROBLEM WITH A NON-LOCAL INTERACTION OF WASSERSTEIN TYPE

JULES CANDAU-TILH AND MARC PEGON

ABSTRACT. We present a numerical study of a non-local isoperimetric problem in $\mathbb{R}^2$ where the perturbation term is defined using the 2-Wasserstein distance. We first investigate the problem restricted to radially symmetric and connected sets. Then, we present numerical simulations obtained by regularizing and discretizing the isoperimetric problem and implementing a gradient descent algorithm. Our results suggest that radial symmetry is lost for large masses. Finally, we detail the implementation of our algorithm, which consists in solving an Allen-Cahn equation by splitting and alternate minimization. The optimal transport term is computed using a variant of the Sinkhorn algorithm.

Keywords and phrases. Nonlocal isoperimetric problems, Wasserstein distance, Allen-Cahn equation, Sinkhorn algorithm, gradient descent, alternate splitting.

2020 Mathematics Subject Classification. 49J45, 90C25, 65K10.

1. INTRODUCTION

In this article, we present some numerical considerations on the non-local isoperimetric problem studied in [8]. Let us denote by W_p the Wasserstein distance for $p \geq 1$ and identify a set $E \subset \mathbb{R}^d$ of finite Lebesgue measure with the restriction $\chi_E \, \mathrm{d}x$ of the Lebesgue measure to E. The non-local energy we consider is the exterior transport functional

$$\mathcal{W}_p(E) = \inf_{|F \cap E| = 0} W_p(E, F),$$

where by convention $W_p(\mu, \nu) = +\infty$ if μ, ν are nonnegative measures with different total mass. Given $\lambda > 0$, we then introduce the variational problem

$$\inf \left\{ P(E) + \lambda \mathcal{W}_p^p(E) : |E| = \omega_d \right\} \tag{1.1}$$

where ω_d is the volume of the unit ball and $P(E)$ denotes the perimeter of E. Let us recall the main results of [8] regarding (1.1). The first one states that solutions do exist and have a bounded number of connected components, all of which being bounded as well:

Theorem 1.1. *For every $d \geq 2$, $p \geq 1$ and $\lambda > 0$, problem (1.1) has minimizers and every minimizer is $\mathcal{H}^{d-1}$-equivalent to a representative set whose boundary is $C^{1,\alpha}$-regular for any $\alpha \in (0, 1/2)$. Moreover, there exists $C = C(d, p) > 0$ such that if $E = \cup_{i=1}^I E^i$ is such a minimizer with E^i the connected components of E, then*

$$\sum_{i=1}^I \operatorname{diam}(E^i) \leq C(1+\lambda)^{d-1} \quad \text{and} \quad \inf_i \operatorname{diam}(E^i) \geq C(1+\lambda)^{-1}.$$

As a consequence $I \leq C(1+\lambda)^d$.

The second theorem of [8] establishes that in the regime where the perimeter is the dominant term, balls are the only minimizers of (1.1):

Theorem 1.2. *For every $d \geq 2$, $p \geq 1$, there exists $\lambda_0 > 0$ such that for every $\lambda \leq \lambda_0$, balls are the only minimizers of (1.1).*

Notice that by scaling (1.1) is equivalent to

$$\inf \left\{ P(E) + \mathcal{W}_p^p(E) : |E| = m \right\} \quad \text{with} \quad m = \lambda^{\frac{d}{p+1}}.$$

In particular, the regime $\lambda \ll 1$ where the perimeter is dominant corresponds to $m \ll 1$, and the case $\lambda \gg 1$ corresponds to $m \gg 1$. Notice that when $\lambda \gg 1$ the exterior transport functional, which strongly disfavours the ball, becomes the dominant term. We actually proved in [9, Theorem 1.3] that the ball was the maximizer of Υ among sets of fixed mass. We thus expect that other geometries emerge in the case $\lambda \gg 1$. To be more specific, we notice that the exterior transport functional favours sets which are thin and with as much mass close to its boundary as possible, so that structures such as strips and annuli may be favoured as λ increases.

For the rest of the article fix $d = p = 2$. Let us first consider the radially symmetric version of (1.1):

$$\inf_E \left\{ P(E) + \lambda \mathcal{W}_2^2(E) : E \text{ radially symmetric and connected, } |E| = \omega_2 \right\}. \tag{1.2}$$

We are interested in answering the following questions:

- How does the geometry of minimizers of (1.1) evolves as m varies in $[0, \infty)$?
- If we restrict the study to Problem (1.2), can we numerically observe the minimizer evolving from a ball to an annulus as m increases?
- Is the transition sharp, or does an intermediate regime exist between the cases $m \ll 1$ and $m \gg 1$?

We perform two types of numerical explorations to address these questions: one in the radially symmetric case, where we compute the energies of the ball and annuli, and another one in the general case for comparison. In the radial case, the simulations are quite accurate and they lead us to formulate the following conjecture:

Conjecture 1.3. *There exist $0 < \lambda_1 < \lambda_2$ (where $\lambda_1 \approx 4.95$ and $\lambda_2 \approx 5.55$) such that:*

- *for $0 \leq \lambda \leq \lambda_1$, the unit disk B_1 is the unique local and global minimizer of (1.2),*
- *for $\lambda > \lambda_1$, (1.2) has two local minimizers : B_1 and an annulus A_{r_λ} where $r_\lambda > 0$,*
- *for $\lambda_1 < \lambda < \lambda_2$, the unit disk B_1 is the only global minimizer of (1.2),*
- *for $\lambda = \lambda_2$, (1.2) has two global minimizers: B_1 and a annulus $A_{r'_\lambda}$ where $r'_\lambda > 0$,*
- *for $\lambda > \lambda_2$, the unique global minimizer of (1.2) is an annulus $A_{r''_\lambda}$ where $r''_\lambda > 0$.*

Let us next introduce our study of the model without any a priori symmetry, which corresponds to the minimization problem:

$$\inf \left\{ P(E) + \lambda \mathcal{W}_2^2(E) : |E| = \omega_2 \right\}. \tag{1.3}$$

To carry out the numerical simulations, we replace the perimeter and Wasserstein functionals in (1.3) by more suitable, smoothed functionals. We use a phase-field method, where the characteristic function χ_E of a set $E \subset \mathbb{R}^2$ is replaced with a function $u : \mathbb{R}^2 \to [0, 1]$ such that $\int u = |E|$.

In this context, we approximate the perimeter term by the classical Modica-Mortola functional (see [15]), defined for $\varepsilon > 0$ and $u \in H^1(\mathbb{R}^2)$ as follows:

$$\mathcal{F}_\varepsilon(u) = 3\varepsilon \int_{\mathbb{R}^2} |\nabla u|^2 + \frac{3}{\varepsilon} \int_{\mathbb{R}^2} u^2(1-u)^2. \tag{1.4}$$

We refer the reader to [4, Section 7] for more details on the Γ-convergence of this functional to the perimeter. We would also like to point out the versatility of such phase-field methods, which may be used in the study of interface dynamics [5], fracture problems [2] or multiphase flows [14].

The exterior transport term is defined for a function $u : \mathbb{R}^2 \to [0, 1]$ by

$$\Upsilon(u) = \inf \left\{ W_2^2(u, v) : v \text{ Lebesgue, } 0 \leq v \leq 1 - u \right\},$$

where we identify u and the measure $u\,\mathrm{d}x$ when no confusion can arise. For numerical purposes, we consider its entropic relaxation Υ_γ. It is given for $\gamma > 0$ by

(1.5)
$$\Upsilon_\gamma(u) = \inf_{\pi \in \mathcal{M}(\mathbb{R}^2 \times \mathbb{R}^2)} \left\{ \int_{\mathbb{R}^2 \times \mathbb{R}^2} |x-y|^2 \mathrm{d}\pi(x,y) + \gamma \mathcal{H}(\pi) : \pi_x = u dx,\ 0 \leq \pi_y \leq (1-u)dy \right\},$$

where the (negative) entropy $\mathcal{H}$ is defined for $\pi \in \mathcal{M}(\mathbb{R}^2 \times \mathbb{R}^2)$ by

$$\mathcal{H}(\pi) = \begin{cases} \int_{\mathbb{R}^2 \times \mathbb{R}^2} \pi(\log(\pi) - 1)\mathrm{d}x\mathrm{d}y & \text{if } \pi \ll dx \otimes dy \text{ and } \pi \geq 0, \\ +\infty & \text{otherwise.} \end{cases}$$

This relaxation is classical in computational optimal transport, due to its ability to quickly compute approximated solutions to various optimal transportation problems (see e.g. [12] and [13, Section 4] for more details). It is also worth pointing out that the algorithm we implement to compute Υ_γ is based on the numerical method described in [6], which was itself based on [17].

Eventually, the problem that we are interested in solving is what we call the Modica-Mortola-entropic approximation of (1.1): given $\lambda, \varepsilon, \gamma > 0$, we consider

$$\inf_u \left\{ \mathcal{E}(u) = 3\varepsilon \int_\Omega |\nabla u|^2 + \frac{3}{\varepsilon} \int_\Omega u^2(1-u)^2 + \lambda \Upsilon_\gamma(u) : u : \Omega \to [0,1], \int_{\mathbb{R}^2} u\,\mathrm{d}x = \omega_2 \right\}. \tag{1.6}$$

Formally, λ represents the 'physical' parameter that models the contribution of the exterior transport term to the total energy, while ϵ and γ are two small approximation parameters.

The ambiant space Ω we consider is the torus $\mathbb{R}^2/L\mathbb{Z}^2$ defined for $L > 0$. We discretize Ω using a regular grid and implement a finite difference scheme to compute each energy term. For the optimization, we use an alternate minimization algorithm and treat the optimal transport term using a variant of the Sinkhorn algorithm.

The chapter is organized as follows. In Section 2, we present the theoretical results and conjectures associated to the study of (1.2). In Section 3, we present the numerical simulations we conducted and compare them to the previous conjectures. In Section 4, we give the proofs and computations on which is based our investigation of Problem (1.2). In Section 5, we detail the transition of the original problem (1.1) to its appproximation (1.6). We also derive the evolution equation we use for the implementation of the gradient descent algorithm. In Section 6, we detail the space discretization of (1.6) and the implementation of the gradient descent in this setting. Eventually, in Section 7 we detail the derivation of the Sinkhorn algorithm we use to solve the problem defined by Υ_γ.

2. Results in the two-dimensional radially symmetric case

We now present some theoretical considerations on Problem (1.2). First notice that due to the non-local nature of optimal transport, obtaining a closed form expression for $\mathcal{W}_2^2(E)$ given a generic shape $E \subset \mathbb{R}^d$ is a very difficult task. However, restricting the study to radially symmetric, connected sets allows for more explicit computations.

Given $0 \leq r_m$, we denote by A_{r_m, r_M} the centered open annulus of mass $\omega_2 = \pi$ with inner radius r_m and outer radius $r_M = \sqrt{1 + r_m^2}$. As the mass is fixed, when no confusion can arise we simply write $A_{r_m, r_M} = A_{r_m}$. Notice that with our notation, the case $r_m = 0$ corresponds to the unit disk $A_{r_m} = B_1$. Given $0 \leq r_m$, for the perimeter we always have

$$P(A_{r_m}) = 2\pi \left(r_m + \sqrt{1 + r_m^2} \right),$$

and we give its graph in Figure 1. The difficulty is to compute

$$\mathcal{W}_2^2(A_{r_m}) = \inf \left\{ W_2^2(A_{r_m}, F) : F \subset \mathbb{R}^2, |F \cap A_{r_m}| = 0 \right\}. \tag{2.1}$$

The following proposition allows us to reduce the study $\mathcal{W}_2^2(A_{r_m})$ to a single variable optimization problem. Its proof is postponed to Section 4.1.

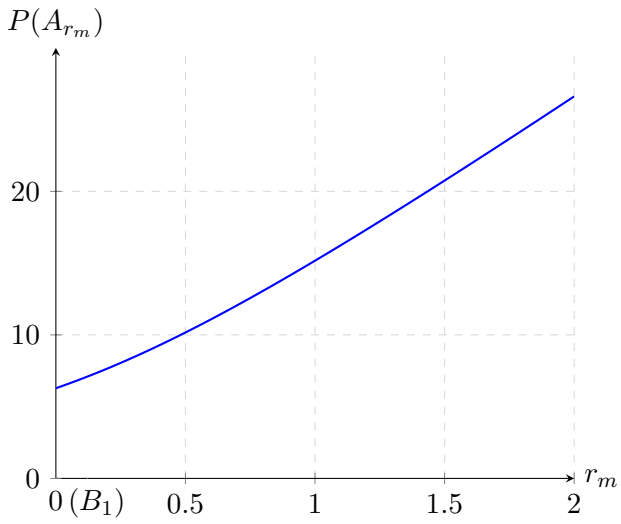

FIGURE 1. Perimeter $P(A_{r_m})$ of the annulus of inner radius r_m.

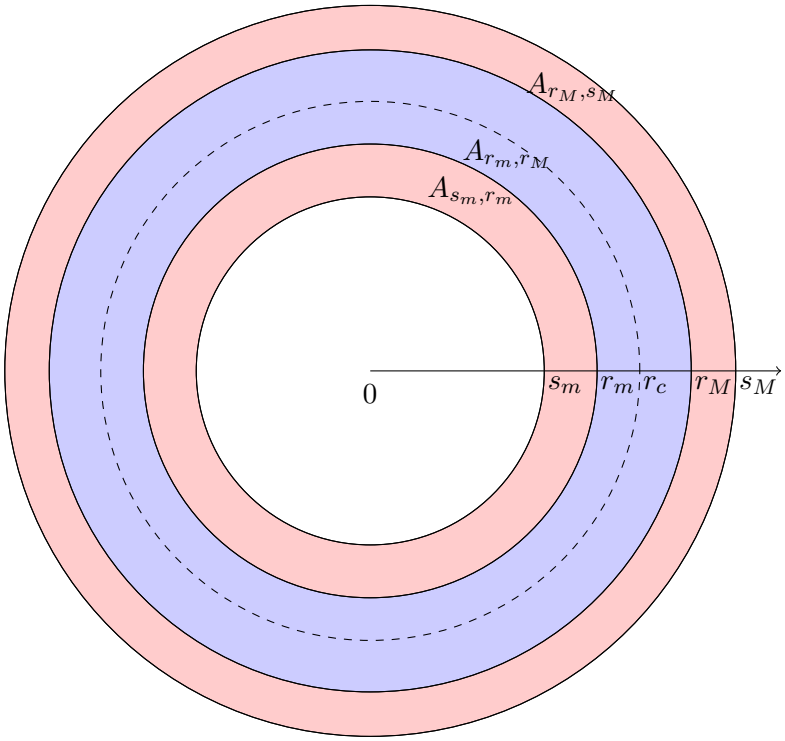

FIGURE 2. The annulus A_{r_m,r_M} and its corresponding minimizer $A_{s_m,r_m} \cup A_{r_M,s_M}$.

Proposition 2.1. *Problem* (2.1) *is uniquely minimized by the reunion F of two annuli adjacent to A_{r_m}, that is*

$$F = A_{s_m,r_m} \cup A_{r_M,s_M},$$

where $0 \le s_m \le r_m$ and $r_M \le s_M$. Additionally, there exists $r_c \in [r_m, r_M]$ such that the optimal exterior transport plan π_{r_c} between A_{r_m} and F is unique and induced by a radially symmetric map $T_{r_c} : \mathbb{R}^2 \to \mathbb{R}^2$. See Figure 2 for an illustration.

The previous proposition gives existence and uniqueness of F and the optimal transport map T_{r_c}, but no way of explicitly computing r_c. For this matter, we exhibit an equation satisfied by

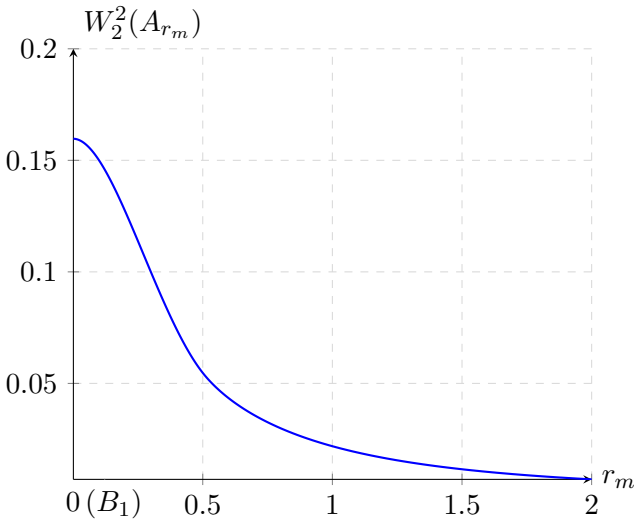

FIGURE 3. Exterior transport energy $W_2^2(A_{r_m})$ of the annulus inner radius r_m.

r_c and then approximate r_c by numerically solving the equation through a secant method. By conservation of the mass, we can then compute s_m and s_M.

First notice that as A_{r_m,r_c} can at most be of mass B_{r_m}, we necessarily have $r_c \leq \sqrt{2}r_m$. For $r_m \leq r_c \leq \hat{r}_M$, with $\hat{r}_M = \min(\sqrt{2}r_m, r_M)$, we denote by $\tau(r_c)$ the transportation cost of sending A_{r_m} to F through the map T_{r_c}. Notice that the value $\hat{r}_M = \sqrt{2}r_m, r_M$ appears because of the fact that the largest possible interior ring is the ball B_{r_m}, implying that $r_c \leq \sqrt{2}r_m$We split $\tau(r_c)$ into $\tau_-(r_c)$ and $\tau_+(r_c)$, which denotes the cost of sending A_{r_m,r_c} (resp. A_{r_c,r_M}) to A_{s_m,r_m} (resp. A_{r_M,s_M}). We have

$$\tau(r_c) = \int_{A_{r_m}} |T_{r_c}(x) - x|^2 \, \mathrm{d}x = \int_{A_{r_m,r_c}} |T_{r_c}(x) - x|^2 \, \mathrm{d}x + \int_{A_{r_c,r_M}} |T_{r_c}(x) - x|^2 \, \mathrm{d}x,$$

and the rest of the computation of τ and τ' is carried out in Section 4.2. We numerically observe that

Assumption 2.2. *The function τ is strictly convex on $[r_m, \hat{r}_M]$ and $\tau'(r_m) < 0$.*

By this assumption, the infimum of τ in $[r_c, \hat{r}_M]$ is reached at some point $\overline{r}_c \in (r_c, \hat{r}_M)$ (exlucing the trivial case of the ball where $\hat{r}_c = r_m = 0$). In practice, we search for $\hat{r}_c$ as follows : we first check if $\tau'(\hat{r}_M) \leq 0$. In this case the minimum is reached at $\hat{r}_M$. Otherwise, we solve $\tau'(r_c) = 0$ for $r_c \in (r_m, \hat{r}_M)$ using a variant of the secant method (see Section 4.3 for the detailed explanation). We thus are able to compute $W_2^2(A_{r_m})$:

$$W_2^2(A_{r_m}) = \inf\left\{\tau(r_c) : r_c \in [r_m, \hat{r}_M]\right\} = \tau(\overline{r}_c), \tag{2.2}$$

whose graph is given in Figure 3.

Eventually, we can compute the energy

$$\mathcal{E}(A_{r_m}) = 2\pi\left(r_m + \sqrt{1 + r_m^2}\right) + \lambda W_2^2(A_{r_m})$$

for different values of $\lambda \geq 0$. Our computations are summarized in Figure 2. We plotted the function $r_m \mapsto \mathcal{E}(A_{r_m})$ for increasing values of $\lambda \geq 0$. Recall that the case $r_m = 0$ corresponds to the unit disk B_1. We added the constant function equals to $\mathcal{E}(B_1)$ on each graph to ease the comparison of the annulus and the disk. Let us point out the fact that these numerical results are correct up to machine accuracy, and that they lead us to make Conjecture 1.3 on the behaviour of the minimizers of 1.2.

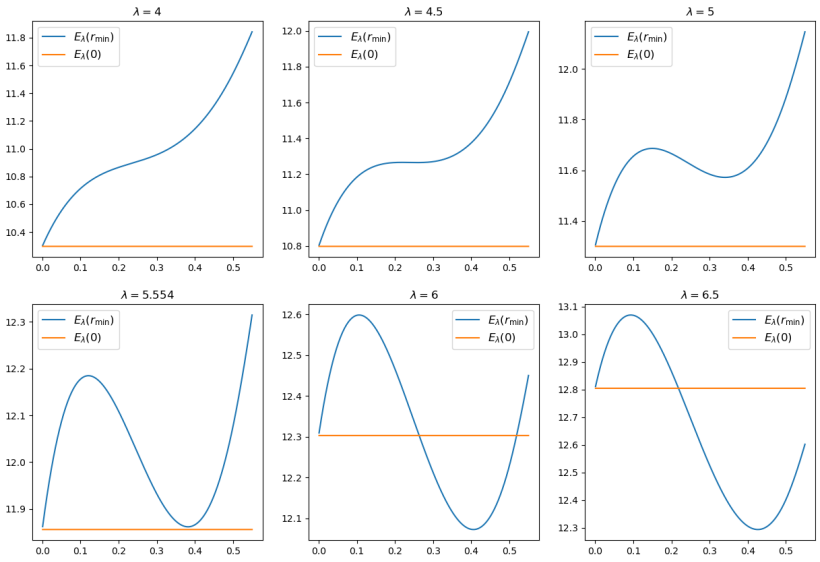

FIGURE 4. Energy of annuli of inner radius r_m and of the disk.

3. Numerical experiments

We now present the results of the numerical experiments conducted in order to study the non radially symmetric problem (1.3). While the detailed implementation of the algorithm is written down in Section 5, let us now briefly summarized it.

3.1. Breakdown of the algorithm.

We work on the torus $\Omega = \mathbb{R}^2/L\mathbb{Z}^2$ that we partition in a regular grid of $N \times N$ squares of side-length $h = L/N$. To solve

$$\inf\left\{\mathcal{E}(u) = \mathcal{F}_\varepsilon(u) + \lambda\Upsilon_\gamma(u),\ u : \Omega \to [0,1],\ \int_\Omega u = \omega_2\right\},$$

we use a gradient descent algorithm. Let us denote by W the double well function $u \mapsto u^2(1-u)^2/2$. Formally computing the first variation of $\mathcal{F}_\varepsilon(u) + \lambda\Upsilon_\gamma(u)$, we obtain the following evolution equation:

$$\partial_t u = 3\varepsilon\Delta u - \frac{3}{\varepsilon}W'(u) + \xi_u + \mu. \tag{3.1}$$

The function ξ_u corresponds to the first variation of Υ_γ, whose detailed computation in our discretized setting is given in Section 7. The real μ is a Lagrange multiplier introduced to encode the preservation of mass. Notice that Equation (3.1) can be seen as an Allen-Cahn equation with a forcing term $\xi_u + \mu$. We then proceed to a Lie splitting and alternatively solve on a time interval of length δ_t:

$$\partial_t u = 3\varepsilon\Delta u \quad \text{and} \quad \partial_t u = -\frac{3}{\varepsilon}W'(u) + \lambda\xi_u + \mu. \tag{3.2}$$

We stop the process when the relative variation of the energy from one iteration to another is inferior to some fixed tolerance thresold. We summarize our notation in the following tabular:

3.2. Presentation of the numerical simulations.

3.2.1. *Comparison of the splitting algorithm and the radial computations.* In this experiment, our goal is to confirm that the limit shapes generated by the splitting algorithm possess energy levels similar to those of the shapes computed in the radially symmetric case. To obtain the set of curves of Figure 3.2.1, we set $L = 4$ and use the splitting algorithm for λ taking sampled values in $[3.5, 7.5]$ and N successively equal to 128, 192 and 256. We initialize the splitting algorithm with a figure U_0 that is already close to be the theoretical optimal figure (i.e. the ball or an optimal annulus) computed in the radially symmetric case. Notice that as N increases, ε

TABLE 1. Parameter values and their descriptions.

Parameter	Description
L	$\Omega = [0, L] \times [0, L] \subset \mathbb{R}^2$ is the grid.
N	Ω is discretized in $N \times N$ squares.
h	$h = L/N$ is the side-length of a square.
ϵ	Modica-Mortola parameter, $\epsilon = 2h$.
γ	Entropic parameter.
λ	The energy is $\mathcal{F}_\epsilon + \lambda \Upsilon_\gamma$.
δ_t	Time step.
tol	Relative tolerance.

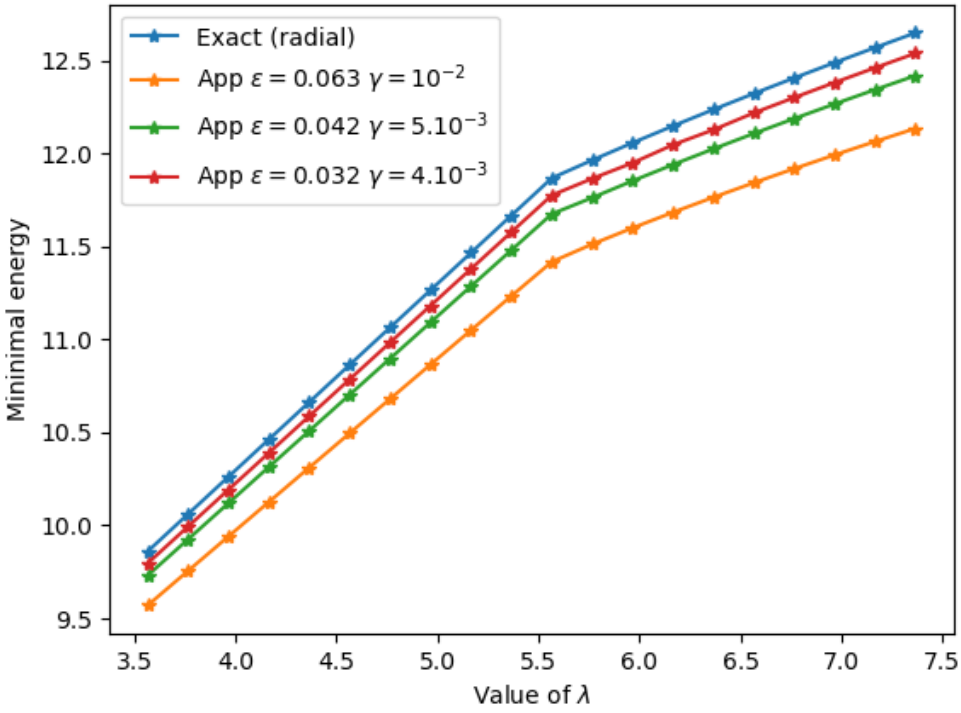

FIGURE 5. Comparison of the 2D model and the radial case

decreases so that we fix decreasing values of γ to have $\gamma \ll \varepsilon$. We fix $\delta_t = \varepsilon/8$ and tol $= 10^{-8}$ in each experiment.

We observe on Figure 2 that the alternate splitting algorithm yields energy values that tends to the ones obtain the computations of the radially symmetric case. Notice that the derivative of the minimal energy with respect to λ has a jump at the critical value $\lambda = \lambda_2 \simeq 5.554$. This corresoponds to the transition from the optimality of the ball to the one of the annulus in the radially symmetric case.

3.2.2. *Stability of the ball and of the annulus.* In this experiment, we set $L = 4$, $N = 256$, $\gamma = 10^{-2}$, tol $= 10^{-8}$ and $\delta_t = \varepsilon/10$ (recall that $\varepsilon = 2h = 2L/N$). In the first simulation, $\lambda = 1$ and we do observe that an non radially symmetric shape close to the ball evolves to the ball. In the second one, $\lambda = 10$ and we start with an annulus. In the limit, we obtain a final annulus close to the optimal one predicted by the radial computations.

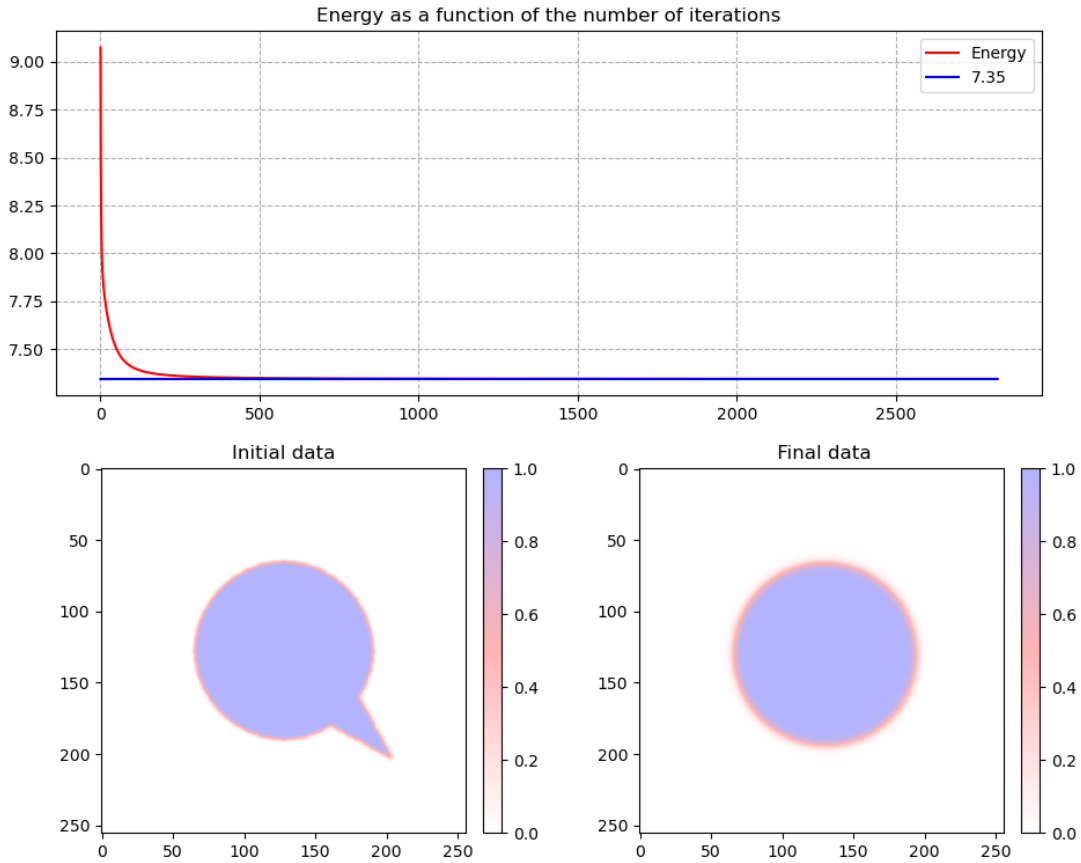

FIGURE 6. Starting with perturbed ball ($\lambda = 1$)

3.2.3. *Some experiments in the critical regime.* In this experiment, we set $L = 4$, $N = 256$, $\gamma = 10^{-2}$, tol $= 10^{-8}$ and $\lambda = \lambda_2 \simeq 5.554$.

This tends to confirm the existence of a critical value λ_2 of λ for which both the disk and some annulus A_{r_m} are global minimizers (see Figure 3.2.3).

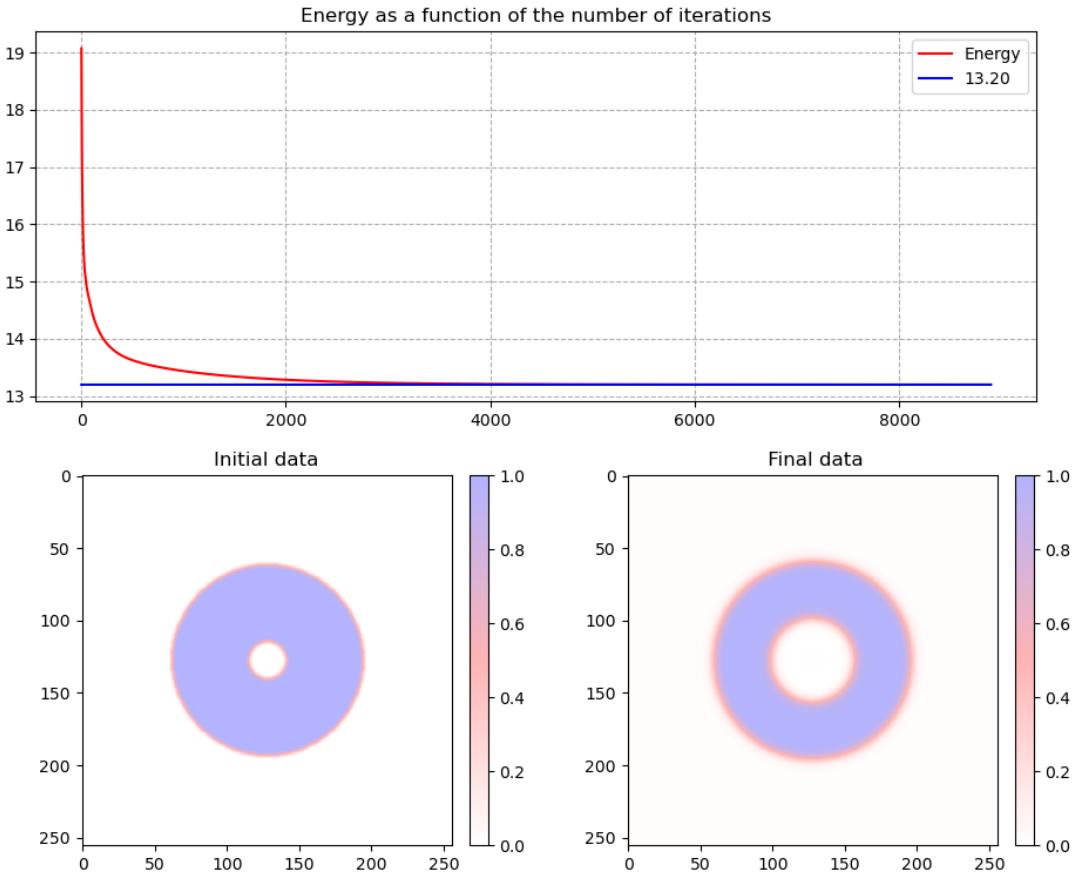

FIGURE 7. Starting with a wide annulus ($\lambda = 10$)

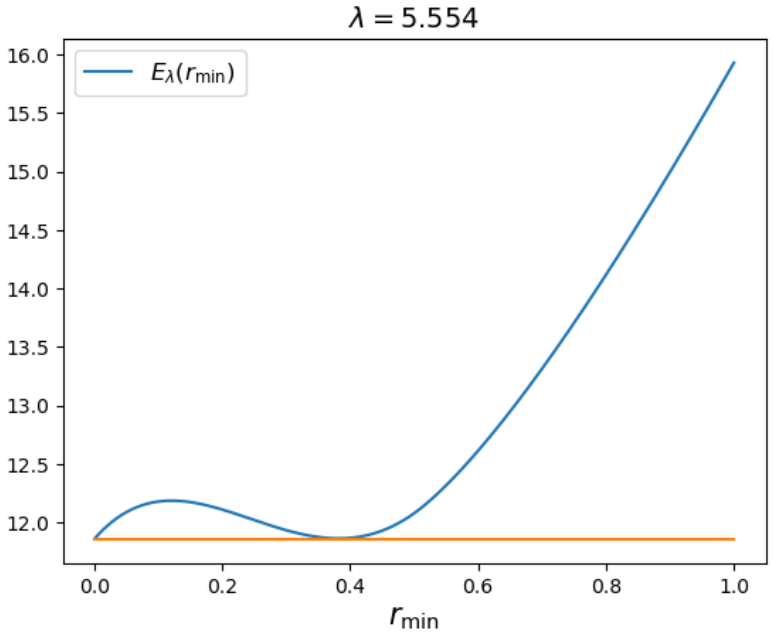

FIGURE 9. Energy of A_{r_m} when r_m varies in the case $\lambda = \lambda_2 \simeq 5.554$.

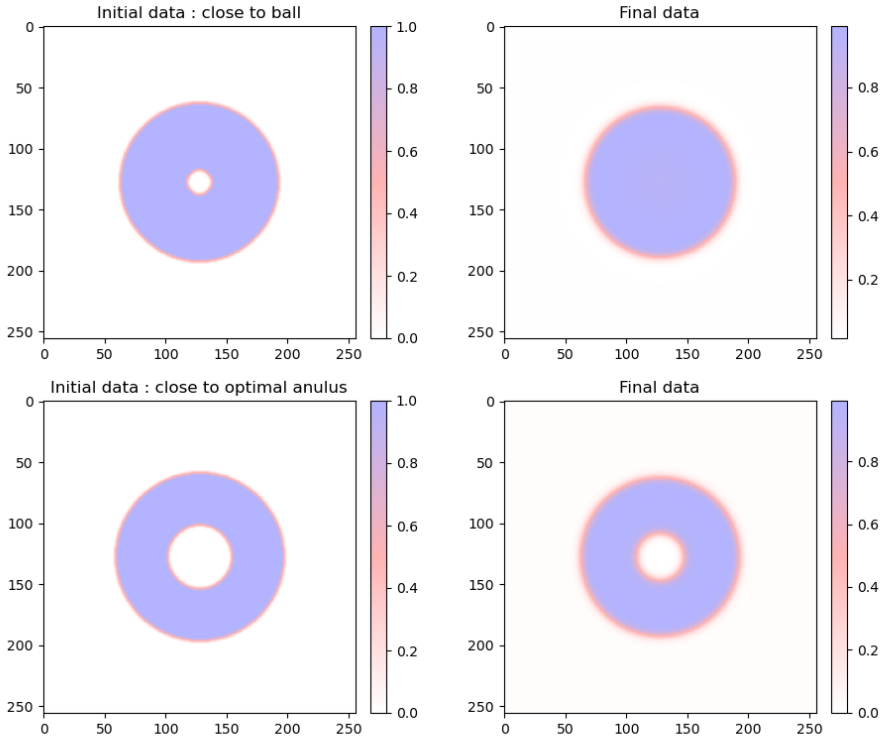

FIGURE 8. Behaviour in the critical regime $\lambda = \lambda_2 \simeq 5.554$.

3.2.4. *Starting away from radially symmetric sets.* When we start with initial data that is highly non radially symmetric, the algorithm struggles to converges to a precisely defined set. Most of the mass uniformly diffuses into the background, while a small set in the center evolves into a disk. To counter this phenomenon, we use a slightly different version of our algorithm, where the mass constraint is more carefully enforced. See Section 6.3 for more details.

In the following experiments we set $L = 8$, $N = 256$, $\gamma = 10^{-2}$, tol $= 10^{-8}$ and $\lambda = 10$.

In those two experiments, we observe that the algorithm does not converge to a radially symmetric figure. Instead, the limit set is elongated and thin and seems to have two axis of symmetry. This leads us to consider the surprising conjecture that thin and elongated shapes are the preferred minimizers as $\lambda \to \infty$, and not annuli.

4. Computation and proofs in the two dimensional radially symmetric case

4.1. **The exterior transport cost functional for a single annulus.**

Proof of Proposition 2.1.

By [8, Proposition 2.1] Problem (2.1) admits a unique minimizer F, and the unique optimal transport plan π between A_{r_m} and F is induced by a map T. By proceeding as in the proof of [8, Lemma 4.2 (i)] we obtain that F is radially symmetric, and eventually that F is the reunion of the two annuli adjacent to A_{r_m} (one of the annuli possibly empty). Regarding the transport map T, it is sufficient to follow the proof of [8, Lemma 4.2 (ii)]. We introduce

$$T_{r_c}(x) = f_{r_c}(|x|)\frac{x}{|x|}, \qquad \text{where} \qquad f_{r_c}(x) = \begin{cases} f_-(x) = \sqrt{s^2 - (r_c - r_m)^2} & \text{if} \quad s \le r_c, \\ f_+(x) = \sqrt{s^2 + (1 + r_m^2 - r_c^2)} & \text{if} \quad s \ge r_c. \end{cases}$$

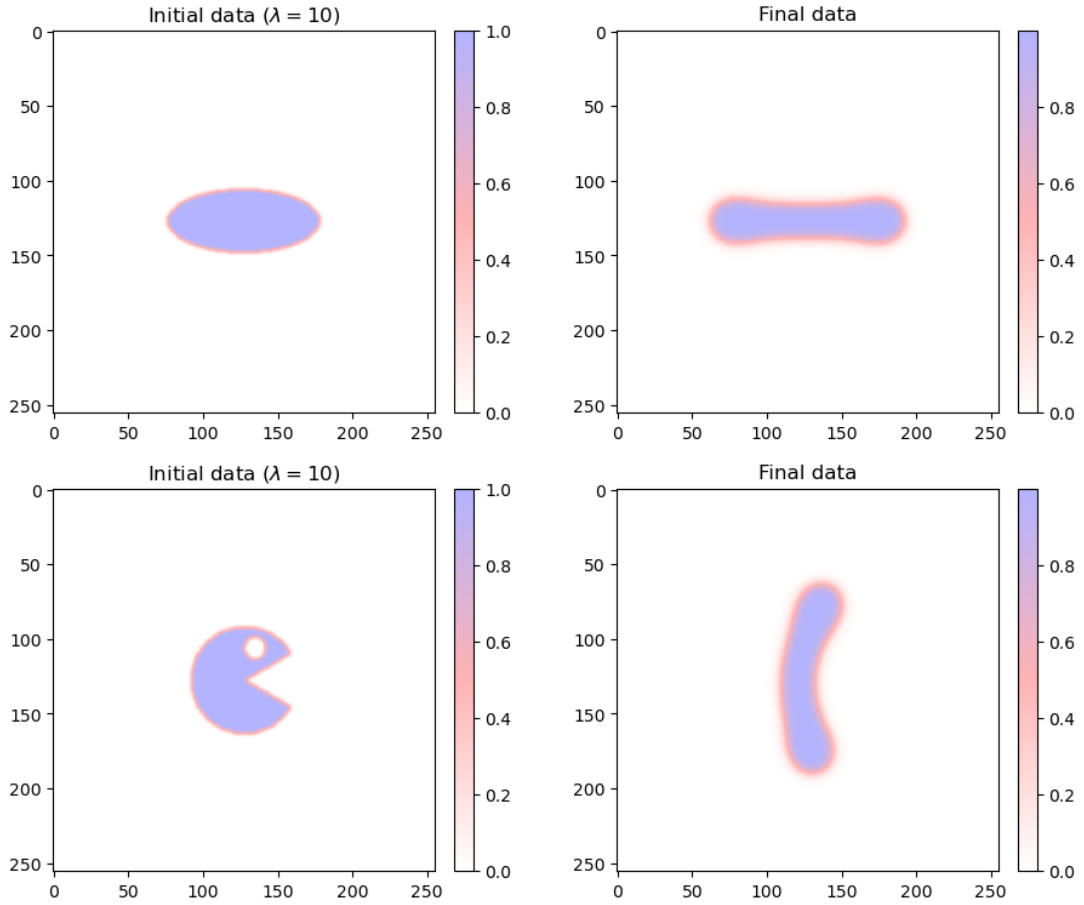

FIGURE 10. Starting with an ellipse and with a pacman ($\lambda = 10$)

Notice that T_{r_c} is the unique radially symmetric map (in the sense that $T(x) = f(|x|)\frac{x}{|x|}$) which solves $\det\nabla T = 1$ and sends A_{r_m} to F. More precisely, T_{r_c} sends A_{r_m,r_c} to A_{s_m,r_m} and A_{r_c,r_M} to A_{r_M,s_M}. As the map

$$g : \mathbb{R}_+ \to \mathbb{R}_+,\ r \mapsto \sqrt{1+r^2}$$

is monotone on $\mathbb{R}_+$, we have that the set $S = \{(x, T(x)) : x \in A_{r_m}\}$ is c-cyclically monotone for the cost $c(x,y) = |x-y|^2$ (see [3, Definition 1.7] for a definition of c-cyclical monotonicity). Therefore, if we define the transport plan $\pi_{r_c} = (\mathrm{Id}, T)_{\#}\chi_{A_{r_m}}\,\mathrm{d}x$, we have that $\mathrm{supp}(\pi_{r_c}) = S$ is c-cyclically monotone. Thus by [3, Theorem 1.13], π_{r_c} is optimal between A_{r_m} and $F = T(A_{r_m})$. Consequently by uniqueness of the optimal transport plan, $\pi = \pi_{r_c}$ and $T = T_{r_c}$. □

4.2. **The splitting radius for the exterior transport of a single annulus.**

Recall that $0 \le r_m$ is fixed, that $\hat{r}_M = \min(r_M, \sqrt{2}r_M)$ and that given $r_c \in [r_m, \hat{r}_M]$, we write $\tau(r_c)$ to denote the cost of transporting A_{r_m} to $A_{s_m,r_m} \cup A_{r_M,s_M}$ by sending A_{r_m,r_c} A_{s_m,r_m} and A_{r_c,r_M} to A_{r_M,s_M} (see Figure 2). Also recall that as a consequence of Proposition 2.1

$$W_2^2(A_{r_m}) = \min\{\tau(r_c) : r_c[r_m, \hat{r}_M] \in\} = \tau(\overline{r}_c),$$

i.e. that the exterior transport problem for A_{r_m} is entirely solved by finding the optimal splitting radius $\overline{r}_c$.

Let us now explain how we obtain an equation on $\overline{r}_c$. We split $\tau(r_c)$ into $\tau_-(r_c)$ and $\tau_+(r_c)$, which denotes the cost of sending A_{r_m,r_c} (resp. A_{r_c,r_M}) to A_{s_m,r_m} (resp. A_{r_M,s_M}). We have

$$\begin{aligned}\tau(r_c) &= \int_{A_{r_m}} |T_{r_c}(x)-x|^2\,\mathrm{d}x = \int_{A_{r_m,r_c}} |T_{r_c}(x)-x|^2\,\mathrm{d}x + \int_{A_{r_c,r_M}} |T_{r_c}(x)-x|^2\,\mathrm{d}x\\ &= \int_{r_m}^{r_c} 2\pi s\Big((s^2-r_c^2+r_m^2)^{1/2}-s\Big)^2\mathrm{d}s + \int_{r_c}^{r_M} 2\pi s\Big((s^2+1+r_m^2-r_c^2)^{1/2}-s\Big)^2\mathrm{d}s.\end{aligned}$$

After integration and denoting by $\delta^2 = r_c^2 - r_m^2$, we have

$$\begin{aligned}\tau_-(r_c) &= \frac{2\pi\delta^2}{4}\ln\left(\frac{r_m+r_c}{r_m+\sqrt{2r_m^2-r_c^2}}\right) + \frac{2\pi\delta^8}{16}\left(\frac{1}{(r_m+r)^4} - \frac{1}{(r_m+\sqrt{2r_m^2-r_c^2})^4}\right),\\ \tau_+(r_c) &= \frac{2\pi(1+\delta^2)^2}{4}\ln\left(\frac{\sqrt{1+r_m^2}+\sqrt{2+2r_m^2-r_c^2}}{\sqrt{1+r_m^2}+r_c}\right)\\ &\quad + \frac{2\pi(1+\delta^2)^4}{16}\left(\frac{1}{(\sqrt{1+r_m^2}+\sqrt{2+2r_m^2-r_c^2})^4} - \frac{1}{(\sqrt{1+r_m^2}+r_c)^4}\right).\end{aligned}$$

By Proposition 2.1, solving (2.1) amounts to finding the unique r_c which minimizes $\tau(r_c)$. First, notice that τ_- is of class C^∞ on $[r_m, \sqrt{2}r_m)$ and of class C^1 on $[r_m, \sqrt{2}r_m]$. The function τ_+ is of class C^∞ on $[r_m, \hat{r}_M]$. Hence τ is of class C^1 on $[r_m, \hat{r}_M]$ and on this interval we compute

$$\begin{aligned}{\tau_-}'(r_c) &= 2\pi r_m r_c\left(2r_m - r_c - \sqrt{2r_m^2-r_c^2}\right) + 2\pi r_c\delta^2\ln\left(\frac{r_m+r_c}{r_m+\sqrt{2r_m^2-r_c^2}}\right),\\ {\tau_+}'(r_c) &= {\tau_{+,1}}'(r_c) + {\tau_{+,2}}'(r_c) + {\tau_{+,3}}'(r_c) + {\tau_{+,4}}'(r_c),\end{aligned}$$

where

$${\tau_{+,1}}' = \frac{\pi(1+\delta^2)}{2}\sqrt{1+r_m^2}\left(\frac{r_c}{\sqrt{2+2r_m^2-r_c^2}} - 1\right),$$

$${\tau_{+,2}}' = -2\pi(1+\delta^2)r_m\ln\left(\frac{\sqrt{1+r_m^2}+\sqrt{2+2r_m^2-r_c^2}}{\sqrt{1+r_m^2}+r_c}\right),$$

$${\tau_{+,3}}' = \frac{\pi(1+\delta^2)^3}{2}\left(\frac{r_m^2+1+r_c^2+2r_c\sqrt{1+r_m^2}}{(\sqrt{1+r_m^2}+r_c)^5}\right),$$

$${\tau_{+,4}}' = -\frac{\pi(1+\delta^2)^3}{2}\left(\frac{3r_m^2+3-r_c^2}{\sqrt{2r_m^2+2-r_c^2}} + 2\sqrt{1+r_m^2}\right)\frac{r_c}{(\sqrt{1+r_m^2}+\sqrt{2r_m^2+2-r_c^2})^5}.$$

Recall that by Assumption 2.2, τ is strictly convex on $[r_m, \hat{r}_M]$ and $\tau'(r_m) < 0$. We then search for the minimum of τ as follows : we first check if $\tau'(\hat{r}_M) \le 0$. In this case the minimum is reached at $\hat{r}_M$. Otherwise, we solve $\tau'(r_c) = 0$ for $r_c \in (r_m, \hat{r}_M)$. We implement a modified secant method described below to find the solution $\overline{r}_c$ to this last equation.

4.3. **A modified secant method to compute the splitting radius.**

Recall that τ_+ is smooth on $[r_m, \hat{r}_M]$ and that τ_- is of class C^1 on $[r_m, \hat{r}_M]$ but not twice differentiable at $\sqrt{2}r_m$. In particular, we have the following asymptotics for τ':

$$\tau'(r_c) = a - b\sqrt{2r_m^2-r_c^2} + O(2r_m^2-r_c^2) \quad \text{for} \quad 0 < \sqrt{2}r_m - r_c \ll 1, \tag{4.1}$$

for some $a \in \mathbb{R}$, $b > 0$ depending on r_m. Following these asymptotics, we implement a modified secant method, where τ' is approximated by some function $f(r_c) = a - b\sqrt{2r_m^2-r_c^2}$ instead of a an affine function $f(r_c) = a + br_c$. Indeed, notice that τ' is not differentiable at $2r_m^2$ and

$\tau' \to +\infty$ as $r_c \to \sqrt{2}r_m$. As a consequence, the classical secant method loses efficiency if the optimal radius $\overline{r}_c$ is close to $\sqrt{2}r_m$.

Now given $a \in \mathbb{R}$ and $b > 0$, we define on $[r_m, \hat{r}_M]$ the function $\eta(a, b, r) = a - b\sqrt{2r_m^2 - r^2}$. In the case where $\tau(\hat{r}_M) > 0$, we initialize the method by setting

$$r[0] = \frac{r_m + r_M}{2} + \frac{r_M - rm}{10}, \quad r[1] = \frac{r_m + r_M}{2} - \frac{r_M - r_m}{10}.$$

Then for $n \geq 1$, we define $a_n \in \mathbb{R}$ and $b_n > 0$ to be such that

$$\eta(a_n, b_n, r[n-1]) = \tau'(r[n-1]) \quad \text{and} \quad \eta(a_n, b_n, r[n]) = \tau'(r[n]). \tag{4.2}$$

Notice that by strict convexity of τ, we have $\tau'(r[n-1]^2) \neq \tau'(r[n])$. We then define $r[n+1]$ to be the solution of $\eta(a_n, b_n, r) = 0$. Solving the system (4.2), we finally obtain that

$$r[n+1] = \left(2r_m^2 - \frac{\left(\tau'(r[n])\sqrt{2r_m^2 - r[n-1]^2} - \tau'(r[n-1])\sqrt{2r_m^2 - r[n]^2}\right)^2}{\left(\tau'(r[n]) - \tau'(r[n-1])\right)^2} \right)^{1/2}. \tag{4.3}$$

We stop the iterations and consider that the method has provided an acceptable approximation for r_c when $|\tau'(r[n+1])| \leq \varepsilon |\tau'(r[1])|$ with $\varepsilon = 10^{-12}$. This secant method thus provides us with a way of computing an approximate value of $\mathcal{W}_2^2(A_{r_m})$ given $r_m \geq 0$.

4.4. **Asymptotic developments of the exterior transport cost.**

Thanks to the numerical simulations, we also notice that there exists r_m^1 such that for $r_m \leq r_m^1$, the entire disk inside A_{r_m} is filled by $A_{s_m, r_m} = B_{r_m}$. In this case, $r_c = \sqrt{2}r_m$, and an expansion at order 5 with respect to $r_m \ll 1$ yields

$$\frac{W_2^2(A_{r_m})}{2\pi} = \frac{\ln(1+\sqrt{2}) + 4 - 3\sqrt{2}}{4} - \frac{\ln(1+\sqrt{2})}{2} r_m^2 + \frac{4\sqrt{2}}{3} r_m^3 + \frac{\ln(1+\sqrt{2}) - 2\sqrt{2}}{2} r_m^4 + \frac{2\sqrt{2}}{15} r_m^5 + O(r_m^6).$$

In the case $r_m \to \infty$, following [16, Appendix B] we expect that r_c admits an a priori expansion of the form

$$\frac{r_c}{r_m} = 1 + \frac{1}{4r_m^2} + \frac{\theta}{16 r_m^4} + O\left(\frac{1}{r_m^6}\right),$$

for some $\theta \in \mathbb{R}$ which we compute by optimizing the quantity $\tau(r_c)$ for fixed $r_m \gg 1$ (we omit the details of this particular optimization). We finally obtain that as $r_m \to \infty$ we have

$$r_c(r_m) = r_m + \frac{1}{4r_m} - \frac{3}{32 r_m^3} + O\left(\frac{1}{r_m^5}\right) \quad \text{and} \quad \frac{W_2^2(A_{r_m})}{2\pi} = \frac{1}{32 r_m^2} - \frac{1}{64 r_m^4} + \frac{67}{6144 r_m^6} + O\left(\frac{1}{r_m^8}\right).$$

5. From the theoretical problem to the numerical implementation

Let us explain how we build approximate solutions of (1.1). For the rest of the article, we will consider that the ambiant space is a compact Ω of $\mathbb{R}^2$ with $|\Omega| \geq 2\omega_2$. Given $\lambda > 0$ we thus aim at solving

$$\inf \Big\{ P(E) + \lambda \Upsilon(E) \ : E \subset \Omega, \, |E| = \omega_d \Big\}.$$

To obtain algorithms that are efficient in terms of computational cost, we substitute each term of the previous problem by an approximate counterpart which is easier to discretize and evaluate.

5.1. **Approximate problem and duality.**

For the perimeter term we use the Modica-Mortola approximation and define $W : \mathbb{R} \to \mathbb{R}$ by

$$W(s) = \frac{1}{2}s^2(1-s)^2 \quad \text{and set} \quad C_W = \int_0^1 \sqrt{2W(s)}\, ds = \frac{1}{6}.$$

Given $\varepsilon > 0$ and $u \in H^1(\Omega)$ we then set

$$\mathcal{F}_\varepsilon(u) = \frac{\varepsilon}{2}\int_\Omega |\nabla u|^2 \,\mathrm{d}x + \frac{1}{\varepsilon}\int_\Omega W(u)\,\mathrm{d}x \quad \text{and.}$$

We denote by $BV(\mathbb{R}^2)$ the set of functions with finite total variation and recall that $\mathcal{F}_\varepsilon$ Γ-converges in $L^1(\Omega)$ (see e.g. [4, Section 7.2] for more details on the Γ-convergence of $\mathcal{F}_\varepsilon$) as $\varepsilon \to 0$ to the functional $\mathcal{F}_0$, where

$$\mathcal{F}_0(u) = \begin{cases} C_W \int_\Omega |\nabla u| \text{ if } u \in \mathrm{BV}(\mathbb{R}^2, \{0,1\}), \\ \infty \quad \text{otherwise.} \end{cases}$$

As for Υ, we follow the usual approach in computational optimal transport and replace it by its entropic approximation (see e.g [10]). By convention we set $0 \log 0 = 0$. The (negative) entropy $\mathcal{H}$ is defined for $\pi \in \mathcal{M}(\Omega \times \Omega)$ by

$$\mathcal{H}(\pi) = \begin{cases} \int_{\Omega\times\Omega} \pi(\log(\pi) - 1)\mathrm{d}x\mathrm{d}y & \text{if } \pi \ll \mathrm{d}x \otimes \mathrm{d}y \text{ and } \pi \geq 0, \\ +\infty & \text{otherwise.} \end{cases}$$

The entropy of a measure $\mu \in \mathcal{M}(\Omega)$ is defined similarly. For $x, y \in \mathbb{R}^d$, let us set $c(x,y) = |x-y|^p$. Given $\gamma > 0$ and $u : \mathbb{R}^d \to [0,1]$ with $\int u = \omega_d$, we define

$$\Upsilon_\gamma(u) = \inf_{\pi \in \mathcal{M}(\Omega\times\Omega)} \left\{ \int_{\Omega\times\Omega} c\mathrm{d}\pi + \gamma\mathcal{H}(\pi) : \pi_x = u\,\mathrm{d}x,\ 0 \leq \pi_y \leq (1-u)\,\mathrm{d}y \right\}. \tag{5.1}$$

A simple application of the Direct Method in the Calculus of Variations allows us to prove the following existence result for (5.1) (which holds for any $p \geq 1$ and $d \geq 2$)

Proposition 5.1. *Let $u : \Omega \to [0,1]$ be such that $\int u = \omega_d$. Assume that there exists at least one exterior transport plan π such that $\mathcal{H}(\pi) < \infty$. Then, the infimum in (5.1) is attained by a unique minimizer $\pi_0 \in \mathcal{M}_+(\Omega \times \Omega)$.*

As a linear optimization problem under convex constraints, given by a linear equality and a linear inequality, (5.1) admits a dual problem. By the Fenchel-Rockafellar theorem, we have:

Proposition 5.2. *Recall that $\Omega \subset \mathbb{R}^d$ is compact. Given $u : \Omega \to [0,1]$ such that $\int u = \omega_d$, we have the following dual formulation for $\Upsilon_\gamma(u)$:*

$$\Upsilon_\gamma(u) = \sup_{\varphi,\psi\in\Phi} \left\{ \int_\Omega u\varphi\,\mathrm{d}x + \int_\Omega (1-u)\psi\,\mathrm{d}y - \gamma\int_{\Omega\times\Omega} e^{\frac{-c+\varphi+\psi}{\gamma}} u(x)\mathrm{d}x(1-u(y))\mathrm{d}y \right\}, \tag{5.2}$$
$$\Phi = \Big\{ (\varphi,\psi) \in C(\Omega)\times C(\Omega),\ \psi \leq 0 \Big\}.$$

Eventually, the problem that we are interested in solving is what we call the Modica-Mortola-entropic approximation of (1.2): given $\varepsilon, \lambda, \gamma > 0$,

$$\inf_u \left\{ \mathcal{E}(u) = 6\mathcal{F}_\varepsilon(u) + \lambda\Upsilon_\gamma(u) : 0 \leq u \leq 1,\ \int u\,\mathrm{d}x = \omega_d \right\}. \tag{5.3}$$

5.2. **Subdifferential of the approximated energy.**

We compute approximate solutions to (5.3) by implementing a gradient descent algorithm. In this regard, we have to exhibit functions belonging the subdifferential of $\mathcal{E}$, which is defined as follows:

$$\partial\mathcal{E}(u) = \left\{ p : \Omega \to \mathbb{R},\ \liminf_{\delta\to 0} \frac{\mathcal{E}(u+\delta(v-u)) - \mathcal{E}(u)}{\delta} \geq p \ \text{ for any } \ v:\ \Omega \to [0,1],\ \int v = \omega_d \right\}.$$

Let us start with the subdifferential of $\mathcal{F}_\varepsilon$. It turns out that we have a stronger result because its first variation is well-known in the literature. Given a functional $\mathcal{G} : L^1(\Omega) \to \mathbb{R}$, we define its first variation in our setting by

$$\delta_u\mathcal{G}(v) = \lim_{\delta\to 0} \frac{\mathcal{G}((1-\delta)u+\delta v) - \mathcal{G}(u)}{\delta} = \lim_{\delta\to 0} \frac{\mathcal{G}(u+\delta(v-u)) - \mathcal{G}(u)}{\delta},.$$

where $u, v : \Omega \to [0,1]$ such that $\int u = \int v = \omega_d$. For the Modica-Mortola functional, we have:

$$\delta_u\mathcal{F}_\varepsilon(v) = -\varepsilon \int_\Omega \Delta u(v-u)\,\mathrm{d}x + \frac{1}{\varepsilon}\int_\Omega W'(u)(v-u)\,\mathrm{d}x, \tag{5.4}$$

with $W'(u) = u(1-u)(1-2u)$.

We now turn to the subdifferential of $\Upsilon_\gamma(u)$. We assume that there exists a couple of potentials (φ_u, ψ_u) maximizing $\Upsilon_\gamma(u)$. Using them as candidates for $\Upsilon_\gamma(u+\delta(v-u))$ and setting $w = v-u$ yield

$$\begin{aligned}\Upsilon_\gamma(u+\delta w) &\geq \int_\Omega \big[u+\delta w\big]\varphi_u\,\mathrm{d}x + \int_\Omega \big[1-(u+\delta w)\big]\psi_u\,\mathrm{d}y \\ &- \gamma\int_{\Omega\times\Omega} \exp\big(\gamma^{-1}\big(-c(x,y)+\varphi_u(x)+\psi_u(y)\big)\big)\big[u(x)+\delta w(x)\big]\big[1-\big(u(y)+\delta w(y)\big)\big]\,\mathrm{d}x\,\mathrm{d}y.\end{aligned}$$

By rearranging the terms and relabeling the integration variables, we recognize that

$$\begin{aligned}\Upsilon_\gamma(u+\delta w) &\geq \Upsilon_\gamma(u) + \delta\int_\Omega(\varphi_u-\psi_u)w\,\mathrm{d}x \\ &- \gamma\,\delta\int_{\Omega\times\Omega} \exp\big(\gamma^{-1}(-c(x,y)+\varphi_u(x)+\psi_u(y))\big)[w(x)(1-u(y)) - w(y)u(x))]\,\mathrm{d}x\,\mathrm{d}y + O(\delta^2).\end{aligned}$$

We finally obtain that

$$\liminf_{\delta\to 0} \frac{\Upsilon(u+\delta w) - \Upsilon_\gamma(u)}{\delta} \geq \int_\Omega(\varphi_u-\psi_u)w\,\mathrm{d}x - \gamma\int_\Omega Gw\,\mathrm{d}x \tag{5.5}$$

where the function G is defined for $x \in \mathbb{R}^d$ by

$$G(x) = \int_\Omega \exp\Big(\frac{-c(x,y)}{\gamma}\Big)\Big[\exp\Big(\frac{\varphi_u(x)+\psi_u(y)}{\gamma}\Big)(1-u(y)) - \exp\Big(\frac{\varphi_u(y)+\psi_u(x)}{\gamma}\Big)u(y)\Big]\,\mathrm{d}y.$$

Combining (5.4) and (5.5), we finally have that the function

$$-6\varepsilon\Delta u + \frac{6}{\varepsilon}W'(u) + \lambda(\varphi_u-\psi_u) - \lambda\gamma G \tag{5.6}$$

belongs to the subdifferential of $\mathcal{E}$. In the numerical implementation of our algorithms, we always have that $\gamma \ll \lambda, \varepsilon$, so that we will omit the last term in (5.6). Consequently, using (5.6) to implement a gradient descent algorithm for $\mathcal{E}$ yields the following evolution equation:

$$\partial_t u = 6\varepsilon\Delta u - \frac{6}{\varepsilon}u(1-u)(1-2u) - \lambda(\varphi_u-\psi_u) + \mu, \tag{5.7}$$

where $\mu \in \mathbb{R}$ is a Lagrange multiplier introduced to encode the preservation of the mass of u. Setting $\xi_u = \varphi_u - \psi_u$, we notice that (5.7) corresponds to an Allen-Cahn equation with an additional term $-\lambda\xi_u + \mu$. Following the notation of [5, Chapter 2], given $t > 0$ we denote by

$S(t)$ the flow of (5.7),
$e^{t\Delta}$ the flow of the diffusion equation $\partial_t u = \varepsilon\Delta u$,

$$Y(t) \quad \text{the flow of the reaction equation} \quad \partial_t u = -\tfrac{1}{\varepsilon} u(1-u)(1-2u) - \lambda \xi_u + \mu,$$

and we approximate $S(t)$ by using the Lie splitting $L(t) = Y(t)e^{t\Delta}$.

6. Space discretization and implementation of the Lie splitting

Let us now describe how we discretize the space $\Omega = [0, L]^2$ and solve each term of the reaction-diffusion equation described just above. In this section, we assume that the term ξ_u related to the exterior transport is known. See the next section for a detailed explanation of how we compute it using a variant of the Sinkhorn algorithm.

6.1. **Solving the diffusion equation by Fourier transform.**

We first have to the classical heat equation on Ω

$$\partial_t u = 6\varepsilon \Delta u.$$

To solve it in a discretized context, we implement a finite difference scheme and use the discrete Fourier transform, which we now comment. Consider the regular partition of Ω into N^2 cubes and identify each cube by a double index (i_1, i_2) with $0 \leq i_1, i_2 \leq N-1$. We specify u to be a function $\overline{u}$ constant on each square of Ω and by abuse of notation identify $\overline{u}$ with the $N \times N$ square matrix of the values it takes. In this context, we compute the discrete partial derivatives of $\overline{u}$ over the x and y axis in the forward fashion, i.e.

$$D_1\,\overline{u}(i_1, i_2) = h^{-1}(\overline{u}(i_1+1, i_2) - \overline{u}(i_1, i_2)) \text{ and } D_2\,\overline{u}(i_1, i_2) = h^{-1}(\overline{u}(i_1, i_2+1) - \overline{u}(i_1, i_2)),$$

where the boundary conditions are periodic: $N - 1 + 1 = 0$ and $N - 1 + 1 = 0$. The equation verified by $\overline{u}$ is then

$$\partial_t \overline{u}(i_1, i_2, t) = \varepsilon \Big[D_1^2 \overline{u}(i_1, i_2, t) + D_2^2 \overline{u}(i_1, i_2, t) \Big]. \tag{6.1}$$

where D^2 corresponds to the forward derivative iterated with the backward one. We can then write $\overline{u}$ as the linear sum of its Fourier coefficients as follows

$$\overline{u}(i_1, i_2, t) = \sum_{k_1=0}^{N-1} \sum_{k_2=0}^{N-1} \mathcal{F}(\overline{u})(k_1, k_2, t) e^{-2\pi i \left(\frac{i_1 k_1}{N} + \frac{i_2 k_2}{N} \right)},$$

Injecting this expression into (6.1), expanding the derivatives and factorizing twice by the half-angle yields

$$\partial_t \mathcal{F}(\overline{u})(k_1, k_2, t) = -4\varepsilon \left(\frac{\sin^2(\pi k_1 h^{-1}) + \sin^2(\pi k_2 h^{-1})}{h^2} \right) \mathcal{F}(\overline{u})(k_1, k_2, t)$$

Solving this equation in $t > 0$ we obtain

$$\mathcal{F}(\overline{u})(t) = e^{\varepsilon C_1 t} \mathcal{F}(\overline{u})(0) \quad \text{where} \quad C_1(k_1, k_2) = -4 \left(\frac{\sin^2(\pi k_1 h^{-1}) + \sin^2(\pi k_2 h^{-1})}{h^2} \right)$$

Inverting the Fourier transform, we finally obtain the following expression for the discretized flow e^{tD} of $e^{t\Delta}$:

$$e^{tD}(\overline{u}_0)(t) = \mathcal{F}^{-1} \left(e^{\varepsilon C_1 t} \mathcal{F}(\overline{u}_0) \right),$$

which we will discretize in time accordingly during the implementation of the algorithm.

6.2. **Solving the reaction equation by the explicit Euler method.**

We now have to solve the following non-linear differential equation

$$\partial_t u = -\frac{6}{\varepsilon} u(1-u)(1-2u) - \lambda \xi_u. \tag{6.2}$$

The discretization and computation of ξ_u is done using a modified Sinkhorn algorithm described in the following section. Now assuming that ξ_u is given, a simple way of approximately solving (6.2) is by the use of an explicit Euler scheme. Given an initial condition u_0, we define u at time $t > 0$ as

$$u(t) = u_0 - t\left(\frac{1}{\varepsilon} u_0(1-u_0)(1-2u_0) + \xi(u_0)\right), \tag{6.3}$$

In the discrete setting, the implementation simply consists in applying (6.3) on each cube of the discretization of Ω.

6.3. **Slight modification of the algorithm for non radially symmetric cases.**

In the first version of the splitting algorithm, our handling of the mass constraint simply amounts to having a step where the missing mass is uniformly distributed over the grid. However, in some situations this process can lead to situations of over-diffusion, where most of the mass of the initial data trivially fades into the background. In order to solve this difficulty, we introduce a second algorithm with an alternative handling of the mass constraint. This corresponds to implementing the second model of the conservative Allen-Cahn equation in [5, Section 3.5] (see also [**BreBra**] on this exact topic).

For the sake of the explanation we assume that $\gamma = 0$. We consider the function $\Phi : [0,1] \to [0,1]$ such that

$$\Phi(s) = 6\int_0^s \sqrt{2W(t)}dt = 6\int_0^s (t-t^2)dt = (3-2s)\,s^2,$$

and a slightly modified version of Problem (5.3):

$$\inf_u \left\{ \overline{\mathcal{E}}(u) = 3\varepsilon \int_\Omega |\nabla u|^2 dx + \frac{1}{\varepsilon}\int_\Omega 6\,W(u)dx + \lambda \Upsilon(\Phi(u)) : 0 \le u \le 1,\ \int_\Omega \Phi(u) = m \right\}.$$

Replacing u by $\Phi(u)$ in the exterior transport term and in the mass constraint yields the following Allen-Cahn equation when computing the first variation of $\overline{\mathcal{E}}$:

$$\frac{\partial_t u}{6} = \varepsilon \Delta u - \frac{1}{\varepsilon} W'(u) - \lambda\sqrt{2W(u)}\xi_u + \sqrt{2W(u)}\mu, \tag{6.4}$$

where $\sqrt{2W(u)}\mu = u(1-u)\mu$ is the Lagrange multiplier encoding the mass constraint. The main purpose of this new phase-field equation is the non-uniformity of the Lagrange multiplier, which allows for a more precise handling of potential mass loss. We also observe that $\Phi(u) = u$ if $u = \chi_E$ for some set $E \subset \Omega$. Consequently, the alternative and classic algorithm coincide as $\varepsilon \to 0$ and the solutions of the Allen-Cahn equation converge to characteristic functions of sets.

7. A modified Sinkhorn algorithm for the entropic exterior transport

In this section, we provide a detailed exposition of the computation of the discretized version of Υ. In particular, we explain how the exterior transport term ξ_u appearing in the reaction step of the Allen-Cahn equation (5.7) is computed. Given $\Omega = [0,L]^2$ as in the previous section, recall that Υ was defined on the set of Borel functions $u : \Omega \to [0,1]$ such that $\int u = \omega_d$ as

$$\Upsilon(u) = \inf_{\pi \in \mathcal{M}_+(\Omega\times\Omega)} \left\{ \int_{\Omega\times\Omega} |x-y|^2 \mathrm{d}\pi : \pi_x = u\,\mathrm{d}x,\ \pi_y \le (1-u)\,\mathrm{d}y \right\}, \tag{7.1}$$

with π_x and π_y being the first and second marginal of π. Given $N \ge 1$, we denote by

$$\mathcal{Q} = \{Q_i\}_{i=1}^{N^2}$$

the collection of N^2 regularly distributed squares partitioning Ω, and set $h = L/N$. In this context, u is a piecewise constant function of the form

$$u = \sum_{i=1}^{N^2} u_i \mathbf{1}_{Q_i} \quad \text{with} \quad u_i \in [0,1] \quad \text{and} \quad \sum_{i=1}^{N^2} u_i h^2 = \omega_d.$$

7.1. **Entropic regularization of the discrete exterior transport problem.**

We now set $n = m = N^2$ and in the rest of the article, we write $\mathbb{R}^n_+$ and $\mathbb{R}^m_+$ to denote respectively the initial and target vector spaces of our exterior optimal transport problem. Let us define $\mathbf{M}^{n,m}_+$ as the convex set of matrices of size $n \times m$ with nonnegative coefficients. Given $1 \leq i \leq n$ and $1 \leq j \leq m$, we denote

$$C = (C_{i,j})_{i,j} = (h^2 |i-j|^2)_{i,j}$$

the cost matrix associated with the 2-Wasserstein distance. We now define $\overline{u}$ to be the vector $(u_1, u_2, \ldots, u_n) \in \mathbb{R}^n_+$ of the values taken by u. Therefore (7.1) rewrites in its discretized form:

$$\inf \Big\{ \langle C, P \rangle \ : P \in \mathbf{M}^{n,m}_+, \ P \mathbb{1}^m = \overline{u}, \ {}^t P \mathbb{1}^n \leq \mathbb{1}^m - \overline{u} \Big\}.$$

Here, $\langle \cdot, \cdot \rangle$ is the canonical inner product of matrices and $\mathbb{1}^n = (1, \ldots, 1) \in \mathbb{R}^n$. To solve this problem numerically, we consider its usual entropic regularization (see [18, Chapter 4]) and consider instead for $\varepsilon > 0$

$$\inf \Big\{ \langle C, P \rangle + \varepsilon H(P) \ : P \in \mathbf{M}^{n,m}_+, \ P \mathbb{1}^m = \overline{u}, \ {}^t P \mathbb{1}^n \leq \mathbb{1}^m - \overline{u} \Big\}, \tag{7.2}$$

where the discrete entropy H is defined as

$$H(P) = \sum_{i,j} P_{i,j} (\log(P_{i,j}) - 1).$$

To quantify the difference between $P \in \mathbf{M}^{n,m}_+$ and a reference kernel $K \in \mathbf{M}^{n,m}_+$ (see [18, Remark 4.2]), we introduce the discrete Kullback–Leibler divergence:

$$KL(P|K) = \sum_{i,j} P_{i,j} \log\left(\frac{P_{i,j}}{K_{i,j}}\right) - P_{i,j} + K_{i,j}.$$

We now set for $1 \leq i \leq n$ and $1 \leq j \leq m$

$$\overline{K} = (\overline{K}_{i,j})_{i,j} = u_i \, e^{-\frac{C_{i,j}}{\varepsilon}} (1 - u_j).$$

Notice that by definition, $KL(P|K) = +\infty$ if $K_{i,j} = 0$ and $P_{i,j} > 0$ for some couple (i,j). Thus when explicitly minimizing (7.2) we can simply set $P_{i,j} = 0$ if $K_{i,j} = 0$ (i.e. if $u_i = 0$ or $u_j = 1$). In what follows, we assume that $u_i > 0$ and $1 - u_j > 0$ for any $1 \leq i \leq n$ and $1 \leq j \leq m$. By direct computation, given $P \in \mathbf{M}^{n,m}_+$ we notice that

$$\varepsilon KL(P|\overline{K}) - \varepsilon \sum_{i,j} \overline{K}_{i,j} = \langle \overline{C}, P \rangle + \varepsilon H(P),$$

where the modified cost $\overline{C} \in \mathbf{M}^{n,m}_+$ is defined as

$$\overline{C}_{i,j} = C_{i,j} - \varepsilon \log(u_i(1-u_j)).$$

Solving (7.2) with $\overline{C}$ thus amounts to minimizing $KL(P|\overline{K})$ with the same constraints on P.

7.2. **Dual formulation of the discrete exterior transport problem.**

As a constrained convex minimization problem, (7.2) admits a dual formulation. We denote by $\mathbb{R}^m_-$ the vectors of $\mathbb{R}^m$ with nonpositive coefficients. Let us introduce the dual variables $f, g \in \mathbb{R}^n \times \mathbb{R}^m_-$ to encode the constraint. We admit that there is no duality gap (see [9, Proposition 3.5] for a proof in a Polish space but with $\gamma = 0$), so that the primal and dual problems coincide. We then compute

$$\begin{aligned}
&\inf\left\{\langle \overline{C}, P\rangle + \varepsilon H(P) \ : P \in \mathbf{M}_+^{n,m},\ P\mathbb{1}^m = \overline{u},\ {}^tP\mathbb{1}^n \leq \mathbb{1}^m - \overline{u}\right\}\\
&= \inf_{P\in\mathbf{M}_+^{n,m}} \sup_{f,g\in\mathbb{R}^n\times\mathbb{R}^m_-} \Big(\langle \overline{C}, P\rangle + \varepsilon H(P) - \langle P\mathbb{1}^m - \overline{u}, f\rangle - \langle {}^tP\mathbb{1}^n - \mathbb{1}^m + \overline{u}, g\rangle\Big)\\
&= \sup_{f,g\in\mathbb{R}^n\times\mathbb{R}^m_-} \inf\nolimits_{P\in\mathbf{M}_+^{n,m}} \Big(\langle \overline{C}, P\rangle + \varepsilon H(P) - \langle P\mathbb{1}^m, f\rangle - \langle {}^tP\mathbb{1}^n, g\rangle\Big) + \langle \overline{u}, f\rangle + \langle \mathbb{1}^m - \overline{u}, g\rangle.
\end{aligned}$$

By convexity of the functions involved,

$$\inf_{P\in\mathbf{M}_+^{n,m}} \Big(\langle \overline{C}, P\rangle + \varepsilon H(P) - \langle P\mathbb{1}^m, f\rangle - \langle {}^tP\mathbb{1}^n, g\rangle\Big)$$

admits a minimizer satisfying

$$\nabla_P\Big(\langle \overline{C}, P\rangle + \varepsilon H(P) - \langle P\mathbb{1}^m, f\rangle - \langle {}^tP\mathbb{1}^n, g\rangle\Big) = 0.$$

Solving this equation we obtain the following expression for P:

$$P_{i,j} = e^{-\frac{\overline{C}_{ij} - (f_i + g_j)}{\varepsilon}}.$$

Injecting it in the last line of (7.2) we obtain a second duality formula:

$$\begin{aligned}
&\inf\left\{\langle \overline{C}, P\rangle + \varepsilon H(P) \ : P \in \mathbf{M}_+^{n,m},\ P\mathbb{1}^m = \overline{u},\ {}^tP\mathbb{1}^n \leq \mathbb{1}^m - \overline{u}\right\}\\
&= \sup_{f,g\in\mathbb{R}^n\times\mathbb{R}^m_-} \left(\langle f, \overline{u}\rangle + \langle g, \mathbb{1}^m - \overline{u}\rangle - \varepsilon \sum_{i,j} e^{-\frac{\overline{C}_{ij} - (f_i + g_j)}{\varepsilon}}\right).
\end{aligned} \tag{7.3}$$

The Sinkhorn algorithm consists in iteratively building approximate solutions of the dual problem in (7.3). To do so, we first solve (7.3) for f considering g is fixed, and then compute g fixing f to be the previously computed value. Precisely, for g fixed we consider

$$\sup_{f\in\mathbb{R}^n} \left(\langle f, \overline{u}\rangle + \langle g, \mathbb{1}^m - \overline{u}\rangle - \varepsilon \sum_{i,j} e^{-\frac{\overline{C}_{ij} - (f_i + g_j)}{\varepsilon}}\right).$$

Computing the criticality condition and using the definition of $\overline{C}$ yield that for $1 \leq i \leq n$

$$u_i - e^{\frac{f_i}{\varepsilon}} u_i \ \sum_j e^{\frac{g_j - C_{ij}}{\varepsilon}} (1 - u_j) = 0,$$

that is (as we assumed $u_i > 0$)

$$f_i = -\varepsilon \log\left(\sum_j e^{\frac{g_j - C_{ij}}{\varepsilon}} (1 - u_j)\right).$$

Next, assuming that f is a constant we solve

$$\sup_{g\in\mathbb{R}^m_-} \left(\langle f, \overline{u}\rangle + \langle g, \mathbb{1}^m - \overline{u}\rangle - \varepsilon \sum_{i,j} e^{-\frac{\overline{C}_{ij} - (f_i + g_j)}{\varepsilon}}\right).$$

and obtain that for $1 \leq j \leq m$ the maximizer exists and is given by

$$g_j = \min\left(0, -\varepsilon \log\left(\sum_i u_i e^{\frac{f_i - C_{ij}}{\varepsilon}}\right)\right).$$

We can now initialize the Sinkhorn algorithm by setting $f^{(0)} = g^{(0)} = 0$ and then compute for $k \geq 0$:

$$f_i^{(k+1)} = -\varepsilon \log\left(\sum_j e^{\frac{g_j^{(k)} - C_{i,j}}{\varepsilon}}(1 - u_j)\right),$$
$$g_j^{(k+1)} = \min\left(0, -\varepsilon \log\left(\sum_i u_i e^{\frac{f_i^{(k+1)} - C_{i,j}}{\varepsilon}}\right)\right).$$

This formulation of Sinkhorn is often referred to as Sinkhorn *in the log domain* (see [18, Remark 4.23]). Usually one instead works with the variables $p_i = \exp(f_i/\varepsilon)$ and $q_j = \exp(g_j/\varepsilon)$. Defining $K = (K_{i,j})_{i,j} = \exp(-C_{i,j}/\varepsilon)_{i,j}$, the alternate minimization then rewrites

$$p^{(k+1)} = \frac{\mathbb{1}^n}{K((\mathbb{1}^m - \overline{u}) \odot q^{(k)})},$$
$$q^{(k+1)} = \min\left(\mathbb{1}^m, \frac{\mathbb{1}^m}{{}^tK(\overline{u} \odot p^{(k+1)})}\right).$$

The division is to be understood as element-wise and $\odot$ denotes the element-wise multiplication. The usual multiplication of a vector X of $\mathbb{R}^n$ by a matrix M of $\mathbb{R}^n \times \mathbb{R}^n$ is simply written MX.

Remark 7.1. Recall that the problem is set in a squared domain $\Omega = [0, L]^2$ partitioned into N^2 cubes of $\mathbb{R}^d$ and that $h = L/N$. In this context, it is possible to significantly speed-up the computation done in the Sinkhorn algorithm by avoiding computing matrices of size $n^2 = N^4$ at each iteration. Let $i, j \in \{1, 2, \ldots, N^2\}$ denote the center of the i-th (resp j-th) cube of the partition. We introduce an x-axis and a y-axis in Ω by writing

$$i = (i_1, i_2) \quad \text{and} \quad j = (j_1, j_2) \quad \text{with} \quad i_1, j_1, i_2, j_2 \in \{0, \ldots, N-1\}$$

so that

$$C(i, j) = (|(i_1 - j_1)h|^2 + |(i_2 - j_2)h|^2).$$

Defining the matrices of $\mathbf{M}_+^{N,N}$

$$K_1 = (K^1_{i_1,j_1}) = e^{-\frac{1}{\varepsilon}((i_1 - j_1)h)^2} \quad \text{and} \quad K_2 = (K^2_{i_2,j_2}) = e^{-\frac{1}{\varepsilon}((i_2 - j_2)h)^2},$$

and seeing $\overline{u}$, p and q as $N \times N$ matrices, the products Kp and $K^T q$ respectively amount to $K^1 p K^2$ and $K^1 q K^2$ (since K^1 and K^2 are symmetric). We denote by $\mathbb{1}^{N \times N}$ the square matrix of size $N \times N$ filled with ones. In the end, the algorithm rewrites

$$p^{(k+1)} = \frac{\mathbb{1}^{N \times N}}{K_1((\mathbb{1}^{N \times N} - \overline{u}) \odot q^{(k)}))K_2},$$
$$q^{(k+1)} = \min\left(\mathbb{1}^{N \times N}, \frac{\mathbb{1}^{N \times N}}{K_1(\overline{u} \odot p^{(k+1)})K_2}\right).$$

Acknowledgments. We are grateful to A. Natale for suggesting the implementation of the Sinkhorn algorithm with the kernel $\overline{K}$ instead of K. While K is typically used to solve the classical optimal transport problem, using $\overline{K}$ simplifies the numerical computations in our non-classical problem.

The authors also wish to thank B. Merlet for several fruitful discussions during the preparation and writing of this chapter.

References

[1] Samuel M. Allen and John W. Cahn. "A microscopic theory for antiphase boundary motion and its application to antiphase domain coarsening". In: *Acta Metallurgica* 27.6 (1979), pp. 1085–1095. ISSN: 0001-6160. DOI: https://doi.org/10.1016/0001-6160(79)90196-2. URL: https://www.sciencedirect.com/science/article/pii/0001616079901962.

[2] Marreddy Ambati, Tymofiy Gerasimov, and Laura De Lorenzis. "A review on phase-field models of brittle fracture and a new fast hybrid formulation". In: *Computational Mechanics* 55 (2 2015), pp. 383–405. DOI: 10.1007/s00466-014-1109-y. URL: https://doi.org/10.1007/s00466-014-1109-y.

[3] Luigi Ambrosio and Nicola Gigli. *A user's guide to optimal transport*. 2009. URL: https://hal.science/hal-00769391.

[4] Andrea Braides. "A Handbook of Γ-convergence". In: *Handb. Diff. Equ.: Stationary Partial Differ. Equ.* 3 (2006), pp. 101–213.

[5] Elie Bretin. "Mouvements par courbure moyenne et méthode de champs de phase". Theses. Institut National Polytechnique de Grenoble - INPG, Apr. 2009. URL: https://theses.hal.science/tel-00995323.

[6] Giuseppe Buttazzo, Guillaume Carlier, and Maxime Laborde. "On the Wasserstein distance between mutually singular measures". In: *Advances in Calculus of Variations* 13.2 (Apr. 1, 2020), pp. 141–154. ISSN: 1864-8266, 1864-8258. DOI: 10.1515/acv-2017-0036. URL: https://www.degruyter.com/document/doi/10.1515/acv-2017-0036/html (visited on 01/03/2022).

[7] John W. Cahn and John E. Hilliard. "Free energy of a Nonuniform system I. Interfacial free energy". In: *J. Chem. Phys.* 28 (1958), pp. 258–267.

[8] Jules Candau-Tilh and Michael Goldman. "Existence and stability results for an isoperimetric problem with a non-local interaction of Wasserstein type". In: *ESAIM: COCV* 28 (2022), p. 37. DOI: 10.1051/cocv/2022040. URL: https://doi.org/10.1051/cocv/2022040.

[9] Jules Candau-Tilh, Michael Goldman, and Benoit Merlet. *An exterior optimal transport problem*. preprint, arXiv: 2309.02806. 2023.

[10] Guillaume Carlier, Vincent Duval, Gabriel Peyré, and Bernhard Schmitzer. "Convergence of Entropic Schemes for Optimal Transport and Gradient Flows". In: *SIAM Journal on Mathematical Analysis* 49.2 (2017), pp. 1385–1418. DOI: 10.1137/15M1050264. eprint: https://doi.org/10.1137/15M1050264. URL: https://doi.org/10.1137/15M1050264.

[11] Patrick L. Combettes and Jean-Christophe Pesquet. "Proximal Splitting Methods in Signal Processing". In: *Fixed-Point Algorithms for Inverse Problems in Science and Engineering*. New York, NY: Springer New York, 2011, pp. 185–212. ISBN: 978-1-4419-9569-8. DOI: 10.1007/978-1-4419-9569-8_10. URL: https://doi.org/10.1007/978-1-4419-9569-8_10.

[12] Marco Cuturi. "Sinkhorn Distances: Lightspeed Computation of Optimal Transport". In: *Advances in Neural Information Processing Systems*. Ed. by C.J. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K.Q. Weinberger. Vol. 26. Curran Associates, Inc., 2013. URL: https://proceedings.neurips.cc/paper_files/paper/2013/file/af21d0c97db2e27e13572cbf59eb343d-Paper.pdf.

[13] Marco Cuturi and Gabriel Peyré. "Computational Optimal Transport: With Applications to Data Science". In: *Found. Trends Mach. Learn.* 11.5-6 (2019), pp. 355–607. ISSN: 1935-8237. DOI: 10.1561/2200000073. URL: http://dx.doi.org/10.1561/2200000073.

[14] David Jacqmin. "Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling". In: *J. of Computat. Phys.* 155.1 (1999), pp. 96–127. ISSN: 0021-9991. DOI: https://doi.org/10.1006/jcph.1999.6332. URL: https://www.sciencedirect.com/science/article/pii/S0021999199963325.

[15] L. Modica and Mortola S. "An esempio di Gamma-convergenza". In: *Bolletino Unione Mat. Ital. B* 14 (1977), pp. 285–299.

[16] Mark A. Peletier and Matthias Röger. "Partial localization, lipid bilayers, and the elastica functional". In: *Arch. Ration. Mech. Anal.* 193.3 (2009), pp. 475–537. ISSN: 0003-9527. DOI: 10.1007/s00205-008-0150-4. URL: https://doi-org.accesdistant.sorbonne-universite.fr/10.1007/s00205-008-0150-4.

[17] Gabriel Peyré. "Entropic Approximation of Wasserstein Gradient Flows". In: *SIAM Journal on Imaging Sciences* 8 (Oct. 2015), pp. 2323–2351. DOI: 10.1137/15M1010087.

[18] Gabriel Peyré, Marco Cuturi, et al. "Computational optimal transport: With applications to data science". In: *Foundations and Trends® in Machine Learning* 11.5-6 (2019), pp. 355–607.

J. C-T.: Univ. Lille, CNRS, UMR 8524, Inria - Laboratoire Paul Painlevé, F-59000 Lille
Email address: jules.candautilh@univ-lille.fr

M.P.: Univ. Lille, CNRS, UMR 8524, Inria - Laboratoire Paul Painlevé, F-59000 Lille
Email address: jules.candautilh@univ-lille.fr