

A monotonic algorithm for the optimal control of the Fokker-Planck equation

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Abstract—Motivated by some crowd motion models in the presence of noise, we consider an optimal control problem governed by the Fokker-Planck equation. We sketch optimality conditions by means of an Hamilton-Jacobi-Bellman equation and we give a monotonic scheme for the numerical approximation of the solution.

I. INTRODUCTION

Our aim is to solve numerically the following optimization problem:

$$\inf E(\rho, v) := \int_0^1 \int_{\mathbb{R}^d} \frac{1}{2} |v(t, x)|^2 \rho(t, x) dx dt + \int_{\mathbb{R}^d} V(x) \rho(1, x) dx \quad (1)$$

governed by the Fokker-Planck equation

$$\partial_t \rho - \varepsilon^2 \Delta \rho + \operatorname{div}(\rho v) = 0 \text{ on } (0, 1) \times \mathbb{R}^d \quad (2)$$

with (given) initial datum $\rho(0, \cdot) = \rho_0$ where ρ_0 is a probability measure on \mathbb{R}^d .

The main motivation for this model comes from macroscopic crowd motion modelling (see the recent papers of Maury and Venel [10] and Buttazzo, Oudet and Jimenez [3]). Let us mention that in the case $\varepsilon = 0$ and if one imposes a prescribed value ρ_1 to $\rho(1, \cdot)$ instead of having a terminal cost in (1), then the minimal value of the cost is exactly the squared 2-Wasserstein distance between ρ_0 and ρ_1 : this is the dynamic formulation of the optimal transportation due to Brenier and Benamou [1]. In [3], Buttazzo, Jimenez and Oudet, building upon Brenier-Benamou formulation, consider the minimization of the sum of the kinetic energy and an additional term taking into account congestion effects (e.g. the integral of ρ^2), the state equation is the continuity equation ($\varepsilon = 0$) and both initial and terminal probabilities ρ_0 and ρ_1 are prescribed. In the model (1)-(2), one looks for the optimal motion of a crowd that is initially distributed according to ρ_0 and whose dynamics is governed by (2). As usual, the diffusion term in (2) amounts to considering that the individual dynamics of particles is governed by a stochastic differential equation with volatility $\sqrt{2}\varepsilon$. The cost functional E that we consider involves the total kinetic energy (as in [1] and [3]) plus a terminal cost given by a potential V . The interpretation of this terminal cost is that

the crowd aims to reach zones of low potential V at the terminal time 1 (as an extreme case, if V is 0 on some set K and $+\infty$ elsewhere then the aim of the crowd is to be in the safe zone K at the terminal time). Some variants and generalizations of this simple model present some similarities with *Mean-Field Games* recently introduced by J.-M. Lasry and P.-L. Lions ([5] [6] [7]).

II. OPTIMALITY CONDITIONS

In this section, we give an informal description of the optimality conditions for the minimization problem (1)-(2) (existence results, detailed proofs and generalizations to a wider class of functionals will be given in [4]). Let us start by remarking, as in Brenier and Benamou [1] that E is convex in the variables $(\rho, m) := (\rho, \rho v)$ and the Fokker-Planck equation is linear in these variables. By a strict convexity argument, there is in fact uniqueness of the minimizer. Let us now note that (2) together with the Cauchy datum $\rho(0, \cdot) = \rho_0$ can be written in the weak form as

$$\int_{\mathbb{R}^d} (\phi(1, x) \rho(1, x) - \phi(0, x) \rho_0(x)) dx = \int_0^1 \int_{\mathbb{R}^d} (\partial_t \phi + \varepsilon^2 \Delta \phi + v \cdot \nabla \phi) \rho dx dt \quad (3)$$

for every $\phi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^d)$. Following Brenier and Benamou [1], we then introduce the Lagrangian:

$$\mathcal{L}(\rho, v, \phi) := E(\rho, v) + \int_0^1 \int_{\mathbb{R}^d} (\partial_t \phi + \varepsilon^2 \Delta \phi + v \cdot \nabla \phi) \rho dx dt - \int_{\mathbb{R}^d} \phi(1, \cdot) \rho(1, \cdot) dx + \int_{\mathbb{R}^d} \phi(0, \cdot) \rho_0 dx$$

and rewrite (1)-(2) as:

$$\inf_{(\rho, v)} \sup_{\phi} \mathcal{L}(\rho, v, \phi). \quad (4)$$

The (formal) dual is obtained by permuting the inf and the sup and the conditions characterizing the saddle-point of \mathcal{L} read as (2) together with:

$$v = -\nabla \phi, \quad (5)$$

$$\partial_t \phi + \frac{1}{2} v^2 + v \cdot \nabla \phi + \varepsilon^2 \Delta \phi = 0, \quad (6)$$

$$\phi(1, \cdot) - V = 0. \quad (7)$$

Thus, at least formally (i.e. ignoring regularity issues), the minimization problem (1)-(2) admits a unique solution (ρ, v) where the optimal velocity is given by $v := -\nabla \phi$ and ϕ

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is the solution of the (backward) Hamilton-Jacobi-Bellman equation:

$$\begin{aligned} \partial_t \phi + \varepsilon^2 \Delta \phi - \frac{1}{2} |\nabla \phi|^2 &= 0, \\ \phi(1, \cdot) &= V. \end{aligned} \quad (8)$$

Now, the optimal density ρ is obtained by solving the Fokker-Planck equation (2) with $v = -\nabla \phi$, which can be done as follows. Considering the stochastic differential equation (assuming ϕ is regular enough):

$$dX_t^x = -\nabla \phi(t, X_t) dt + \sqrt{2\varepsilon} dB_t, \quad X_0^x = x \quad (9)$$

(where $(B_t)_t$ is the standard Brownian motion) then it is a well-known consequence of Itô's lemma that $\rho(t, \cdot)$ is the probability law of X_t whenever X_0 is distributed according to the probability ρ_0 , which more precisely means

$$\int_{\mathbb{R}^d} \psi(x) \rho(t, x) dx = \int_{\mathbb{R}^d} \mathbb{E}(\psi(X_t^x)) \rho_0(x) dx \quad (10)$$

for every test-function ψ . The description above deals with the problem (1)-(2) on the whole space. In the whole space, Eq.(8) can be solved explicitly since, using the Hopf-Cole transformation, it reduces to the heat equation.

In our numerical simulations, we will focus on the case of a bounded domain Ω (which requires to consider additional boundary conditions like the Neumann homogeneous boundary conditions $v \cdot n = 0$ in (2) and $\partial_n \rho = 0$ in (8) on $(0, 1) \times \partial\Omega$). In this case, the corresponding Hamilton-Jacobi-Bellman equation does not admit a closed-form solution.

III. DISCRETE SETTING

Before presenting the optimization algorithm, we introduce the following discretization of the problem. Even if what follows easily generalizes to 2D and 3D situations, we will focus in the rest of that paper on the 1D-case for the sake of simplicity. Given a matrix C , we denote by C^* its transpose matrix.

Let us consider two positive integers M, N and a positive real number L . We consider here the case of the bounded space domain $[0, L]$ for (2). We define the time and space steps by $\Delta t = \frac{1}{N}$ and $\Delta x = \frac{L}{M}$ and denote for $j = 0, \dots, M$, $i = 0, \dots, N$ by ρ_j^i and ρ_j the numerical approximations of $\rho(i \cdot \Delta t, j \cdot \Delta x)$ and $\rho(\cdot, j \cdot \Delta x)$ respectively. For reasons that will appear later, the discrete velocity is defined at the points $(i \cdot \Delta t, (j + 1/2) \cdot \Delta x)$, and is therefore denoted by $v_{j+1/2}^i$. To be consistent with the fact that the total mass of $[0, L]$ is constant in time, at the discrete level, we impose the homogeneous Neumann boundary condition for ρ complemented by $v_{1/2}^i = v_{M-1/2}^i = 0$, for $i = 0 \dots N - 1$. We shall also use the notations $v^i = (v_{j+1/2}^i)_{j=0 \dots M-1}$ and $\rho^i = (\rho_j^i)_{j=1 \dots M-1}$.

A. Discretized cost functional

From now on, v stands for the discrete velocity $(v_{j+1/2}^i)_{i,j}$ and V is the vector of components $V_j = V(j \cdot \Delta x)$. We

consider the following discrete version of the cost functional E :

$$\begin{aligned} E_{\Delta t, \Delta x}(v) &:= \Delta t \cdot \Delta x \sum_{i=0}^{N-1} \sum_{j=1}^{M-1} \frac{1}{2} q_j(v^i) \rho_j^i \\ &\quad + \Delta x \sum_{j=1}^{M-1} V_j \rho_j^N \\ &= \Delta t \sum_{i=0}^{N-1} \frac{1}{2} \langle \rho^i, q(v^i) \rangle + \langle \rho^N, V \rangle \end{aligned}$$

where $\langle \cdot, \cdot \rangle$ is the scalar product on \mathbb{R}^{M-1} defined by:

$$\langle u, v \rangle = \Delta x \sum_{j=1}^{M-1} u_j v_j.$$

The vector $q(v^i) = (q_j(v^i))_{j=1 \dots M-1}$ is defined from v^i by:

$$q_j(v^i) = \frac{(v_{j-1/2}^i)^2 + (v_{j+1/2}^i)^2}{2}.$$

This choice corresponds to use a trapezoid rule to approximate $|v|^2$ in the first integral of (1).

B. Numerical scheme for the Fokker-Planck equation

The preservation of the positivity of ρ at the discrete level appears in numerical simulation as a crucial issue, especially for small values of ε . Indeed, the linearity of E with respect to ρ leads to numerical instabilities when using schemes which do not possess this property, independently of their order of accuracy. This fact motivates the use of a low order Godunov scheme for the advective part of (2) which ensures both small computational cost and positivity of the numerical solutions.

Remark 1: In addition, this framework enables us to avoid the introduction of Lagrange multipliers corresponding to the constraint $\rho \geq 0$.

We are now in the position to define the numerical solver of (2). Starting from $\rho_j^0 = \rho_0(j \cdot \Delta x)$, ρ_j^i is computed iteratively for $j = 1 \dots M - 1$ by:

$$\begin{aligned} \rho_j^{i+1} &= \rho_j^i + \varepsilon^2 \frac{\Delta t}{\Delta x^2} (\rho_{j+1}^i - 2\rho_j^i + \rho_{j-1}^i) \\ &\quad - \frac{\Delta t}{\Delta x} (\rho_{j+1/2}^i v_{j+1/2}^i - \rho_{j-1/2}^i v_{j-1/2}^i). \end{aligned} \quad (11)$$

In this equation, the terms $\rho_{j+1/2}^i$ and $\rho_{j-1/2}^i$ of the advective part are defined according to a Godunov scheme, i.e. using up-winding:

$$\rho_{j+1/2}^i = \begin{cases} \rho_{j+1}^i & \text{if } v_{j+1/2}^i < 0 \\ \rho_j^i & \text{if } v_{j+1/2}^i \geq 0. \end{cases}$$

To simplify our notations, we rewrite (11) as:

$$\rho^{i+1} = (A + B(v^i)) \rho^i,$$

where A corresponds to the identity matrix plus the discrete Laplace operator, i.e. the first two terms of the right hand-side of (11), and B is associated to the advective part, i.e. the last term of the right hand-side of (11).

Given a positive vector ρ^i , it is a simple matter to check that a sufficient condition to guarantee the positivity of ρ^{i+1} (and the stability of the scheme) is:

$$\forall j = 1 \dots M-1, |v_{j+1/2}^i| \leq \lambda := \frac{\Delta x}{2\Delta t} - \varepsilon^2 \frac{1}{\Delta x}. \quad (12)$$

IV. OPTIMIZATION PROCEDURE

In order to compute efficiently a minimizing sequence, we use a so called *monotonic scheme*. This approach has already shown a great efficiency in the field of optimal quantum control [8], [9], [12], where gradient methods usually lead to numerical instabilities. These types of algorithms apply for bilinear control problems and are based on a special factorization of the variations in $E_{\Delta t, \Delta x}$ that is presented in the next sections.

A. Adjoint state

In the approach we follow, a crucial role is played by the *adjoint state* $\phi^i = (\phi_j^i)_{j=1 \dots M-1}$ that is defined iteratively for $i = 0 \dots N$, by the backward propagation:

$$\begin{aligned} \phi^N &= V, \\ \phi^i &= (A^* + B^*(v^i))\phi^{i+1} + \frac{\Delta t}{2}q(v^i). \end{aligned} \quad (13)$$

This variable is the discrete version of the Lagrange multiplier defined by (5-7).

B. Variations in $E_{\Delta t, \Delta x}$

We present now the algebraic manipulations at the heart of the monotonic schemes. Let us consider two controls v and v' and the corresponding solutions $(\rho^i)_{i=0 \dots N}$ and $(\rho_j^i)_{i=0 \dots N}$ of (11). In what follows, the adjoint $\phi = (\phi_i)_{i=0 \dots N}$ corresponds to v . One has:

$$\begin{aligned} E_{\Delta t, \Delta x}(v') - E_{\Delta t, \Delta x}(v) &= \frac{\Delta t}{2} \sum_{i=0}^{N-1} \langle \rho^i, q(v^i) - q(v^i) \rangle \\ &\quad + \frac{\Delta t}{2} \sum_{i=0}^{N-1} \langle \rho^i - \rho^i, q(v^i) \rangle \\ &\quad + \sum_{i=0}^{N-1} \langle \rho^{i+1} - \rho^{i+1}, \phi^{i+1} \rangle - \langle \rho^i - \rho^i, \phi^i \rangle \\ &= \frac{\Delta t}{2} \sum_{i=0}^{N-1} \langle \rho^i, q(v^i) - q(v^i) \rangle \\ &\quad + \sum_{i=0}^{N-1} \langle (B(v^i) - B(v^i))\rho^i, \phi^{i+1} \rangle. \end{aligned}$$

This identity can also be expressed locally through the formula:

$$E_{\Delta t, \Delta x}(v') - E_{\Delta t, \Delta x}(v) = \Delta t \cdot \Delta x \sum_{i=0}^{N-1} \sum_{j=1}^{M-2} \Delta_j^i(v', v),$$

where:

$$\begin{aligned} \Delta_j^i(v', v) &= \frac{\rho_j^i + \rho_{j+1}^i}{2} \left(\frac{(v_{j+1/2}^i)^2 - (v_{j+1/2}^i)^2}{2} \right) \\ &\quad + \left(\rho_{j+1/2}^i v_{j+1/2}^i - \tilde{\rho}_{j+1/2}^i v_{j+1/2}^i \right) \left(\frac{\phi_{j+1}^{i+1} - \phi_j^{i+1}}{\Delta x} \right). \end{aligned} \quad (14)$$

In this equation, we have introduced

$$\tilde{\rho}_{j+1/2}^i = \begin{cases} \rho_{j+1}^i & \text{if } v_{j+1/2}^i < 0 \\ \rho_j^i & \text{if } v_{j+1/2}^i \geq 0. \end{cases}$$

Remark 2: Given v , note that the value of $\rho_{j+1/2}^i$ depends on the sign of $v_{j+1/2}^i$, so that $v_{j+1/2}^i \mapsto \Delta_j^i(v', v)$ is a continuous, piecewise polynomial function.

C. Optimization strategy

This section provides a brief exposition of the optimization strategy we follow to solve our problem.

Given v and a positive real number θ , We define $v_{j+1/2}^i$ as a solution of

$$\Delta_j^i(v', v) = -\theta \frac{\rho_j^i + \rho_{j+1}^i}{2} (v_{j+1/2}^i - v_{j+1/2}^i)^2. \quad (15)$$

According to Remark 2, this equation may have one, two or four roots, including the trivial one $v_{j+1/2}^i = v_{j+1/2}^i$. When possible, we define $v_{j+1/2}^i$ as the root of (15) that is closer to $v_{j+1/2}^i$, and we set $v_{j+1/2}^i = v_{j+1/2}^i$ otherwise. Thus, the monotonicity of our algorithm is guaranteed.

Let us give the explicit formula corresponding to this procedure. We suppose that $\frac{\rho_j^i + \rho_{j+1}^i}{2} > 0$, otherwise the contribution of this term is zero for all choice of $v_{j+1/2}^i$. We introduce

$$\delta = \frac{2}{\theta + 1},$$

$$\nu_{j+1/2}^i = \frac{2\tilde{\rho}_{j+1/2}^i}{\rho_j^i + \rho_{j+1}^i},$$

and

$$\tilde{\nu}_{j+1/2}^i = \frac{2\tilde{\rho}_{j+1/2}^i}{\rho_j^i + \rho_{j+1}^i},$$

with

$$\tilde{\rho}_{j+1/2}^i = \begin{cases} \rho_{j+1}^i & \text{if } \tilde{\rho}_{j+1/2}^i = \rho_j^i \\ \rho_j^i & \text{if } \tilde{\rho}_{j+1/2}^i = \rho_{j+1}^i \end{cases}.$$

Consider now:

$$\begin{aligned} \alpha_{j+1/2}^i &= (1 - \delta)v_{j+1/2}^i + \delta\nu_{j+1/2}^i \frac{\phi_{j+1}^{i+1} - \phi_j^{i+1}}{\Delta x}, \\ \beta_{j+1/2}^i &= \\ &= \frac{-b_{j+1/2}^i - \text{sign}(v_{j+1/2}^i) \sqrt{(b_{j+1/2}^i)^2 - 4a_{j+1/2}^i c_{j+1/2}^i}}{2a_{j+1/2}^i}, \end{aligned}$$

where sign is the function

$$\text{sign}(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ -1 & \text{if } x < 0, \end{cases}$$

and :

$$\begin{aligned} a_{j+1/2}^i &= 1 + \theta, \\ b_{j+1/2}^i &= -2(\theta v_{j+1/2}^i + \nu_{j+1/2}^i \frac{\phi_{j+1}^{i+1} - \phi_j^{i+1}}{\Delta x}), \\ c_{j+1/2}^i &= \theta(v_{j+1/2}^i)^2 + \tilde{\nu}_{j+1/2}^i \frac{\phi_{j+1}^{i+1} - \phi_j^{i+1}}{\Delta x}. \end{aligned}$$

The control v_j^i can be expressed by :

$$v_{j+1/2}^i = \begin{cases} \alpha_{j+1/2}^i & \text{if } v_{j+1/2}^i \cdot \alpha_{j+1/2}^i \geq 0 \\ \beta_{j+1/2}^i & \text{if } v_{j+1/2}^i \cdot \alpha_{j+1/2}^i < 0. \end{cases} \quad (16)$$

D. Constraints on v

We recall that the bound (12) on the velocity v is crucial for the positivity of the density. As the stability of our optimization scheme is based on the positivity of the variable ρ , the strategy presented in the last section has to include a slop-limiter such that (12) prevails. Instead of defining $v_{j+1/2}^i$ through (16), we alternatively denote by $\tilde{v}_{j+1/2}^i$ the value obtained in (16) and consider the definition:

$$v_{j+1/2}^i = \text{sign}(\tilde{v}_{j+1/2}^i) \cdot \min(\lambda, |\tilde{v}_{j+1/2}^i|). \quad (17)$$

It is easy to check that this modification does not spoil the monotonicity of our procedure, as soon as v satisfies (12).

E. Algorithm

We can now define precisely our optimization algorithm. Suppose that v^k is given. The computation of v^{k+1} is achieved as follows.

- Define ϕ^k by (13) with $v = v^k$.
- Define $\rho^0 = \rho_0$ and compute iteratively ρ^i from ρ^{i-1} according to the sub-steps:
 - define $(v^{k+1})^{i-1}$ by (17) where $\tilde{v}_{j+1/2}^i$ is computed with $\phi = \phi^k$,
 - define $(\rho^{k+1})^i$ by (11) with $v^{i-1} = (v^{k+1})^i$.

A possible termination criterion is obtained by checking the discrete optimality conditions, i.e., given a tolerance threshold $\text{Tol} > 0$:

$$\sup_{1 \leq i \leq N-1, 1 \leq j \leq M-1} \left(\left| \frac{(\rho^k)_j^i + (\rho^k)_{j+1}^i}{2} (v^k)_{j+1/2}^i + (\rho^k)_{j+1/2}^i \frac{(\phi^k)_{j+1}^{i+1} - (\phi^k)_j^{i+1}}{\Delta x} \right| \right) \leq \text{Tol}. \quad (18)$$

Remark 3: Note that the necessity of the computation of ρ only comes from the Godunov scheme. Indeed, the formal gradient of the Lagrangian with respect to v is:

$$\nabla_v \mathcal{L}(\rho, v, \phi) = \rho(v + \nabla \phi),$$

so that only v and ϕ are necessary to determine the descent direction. This additional computation substitutes the computation of a Lagrange multiplier associated to the positivity constraint that applies on ρ .

V. NUMERICAL RESULTS

This section aims at presenting some numerical results obtained with our approach. In our algorithm we choose $\theta = 1$.

Numerical simulations exhibit very good convergence results. This is explained by the fact that the discrete energy $E_{\Delta t, \Delta x}$ decreases with the iterations of our algorithm and by the strict convexity of E in the variables $(\rho, \rho v)$ which yields uniqueness of the minimizer characterized by the conditions of section II.

A. The 1D-case

We first focus on the computation of optimal transportation between two Gaussian densities in $\Omega = [0, 1]$. We choose:

$$V(x) = 5(1 - e^{-10(x-0.2)^2} - e^{-10(x-0.8)^2}).$$

In a first example, the initial probability is symmetric with respect to space and defined by :

$$\rho(0, x) = e^{-10(x-0.5)^2}.$$

A second test is done with a initial condition that has been slightly shifted to the right. These two results are obtained with $\varepsilon = 0$. The case $\varepsilon > 0$ is treated in a third test.

These functions and the final state are represented in Fig. 1. A fast convergence is observed. In the framework we work,

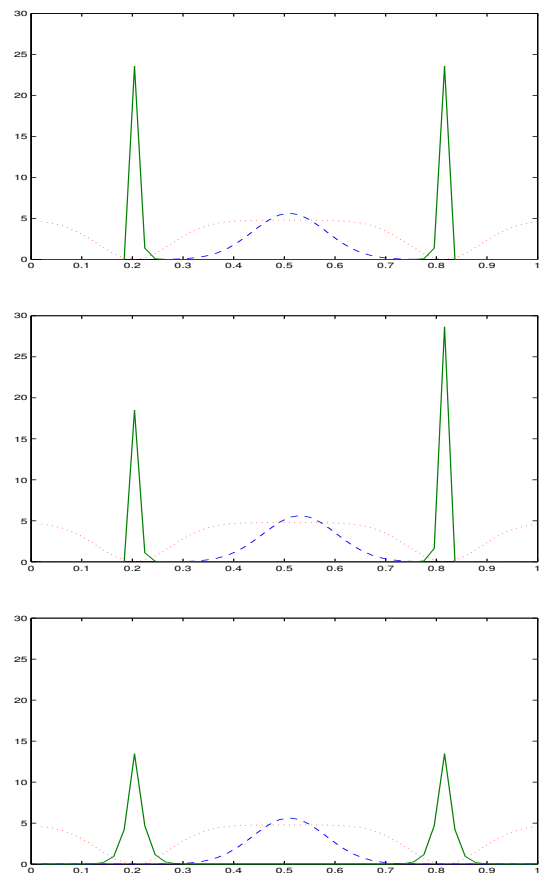


Fig. 1. Evolution of ρ in the 1D-case. Dashed line : initial datum, solid line : final probability, dotted line : potential. Top: symmetric initial probability. Middle: slightly shifted initial probability. Bottom: case $\varepsilon^2 = 10^{-2}$.

the control v has $5 \cdot 10^4$ components. Only 100 iterations, and a CPU time¹ of 196.64s are required to obtain numerical convergence. The cost functional values together with the termination criterion defined in (18) are depicted in Fig. 2.

¹The computation are done using the free software OCTAVE (<http://www.octave.org>).

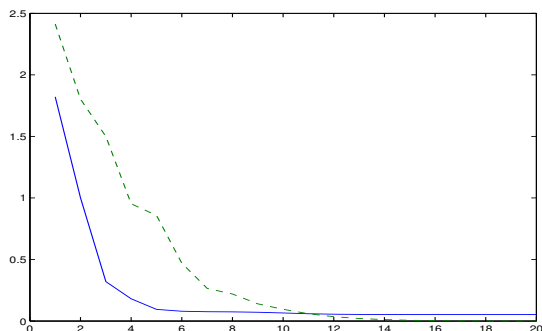


Fig. 2. Numerical convergence in the 20 first iterations. Solid line : Values of $E_{\Delta t, \Delta x}$. dashed line : values of the termination criterion defined in (18) (rescaled).

B. The 2D- case

The algorithm is tested in the 2-dimensional case, with $\Omega = [0, 1] \times [0, 1]$. We consider the initial probability :

$$\rho(0, x, y) = e^{-10(x-0.2)^2} + e^{-10(y-0.2)^2},$$

and the potential :

$$V(x, y) = 40(1 + e^{-10(y-0.8)^2} - e^{-10(x-0.8)^2} + e^{-10(y-0.5)^2} - e^{-10(x-0.5)^2}).$$

This potential is represented in Fig. 3. The evolution of the

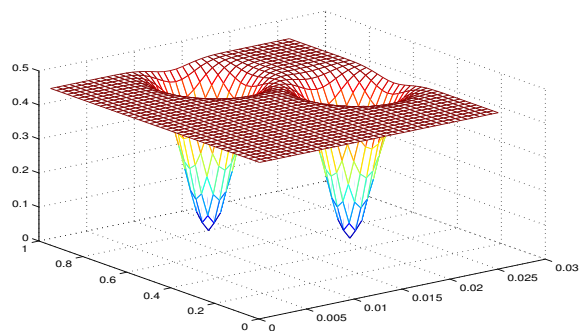


Fig. 3. Potential $V(x, y)$.

probability ρ during the transportation is depicted in Fig. 4. As it was the case in 1D, the numerical convergence is obtained in about 100 iterations.

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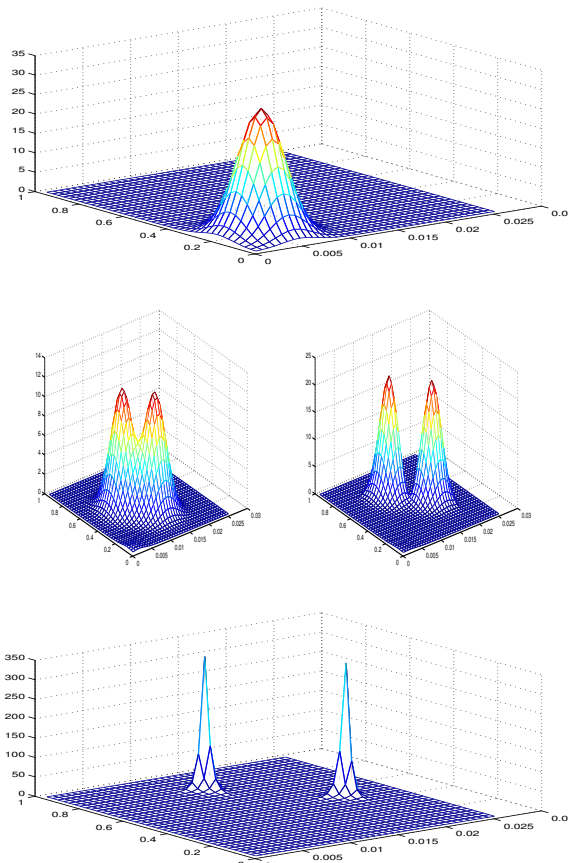


Fig. 4. Evolution of ρ in the 2D-case. Top: initial probability. Middle: probability at time $t = .5$ and $t = .75$. Bottom: final probability.

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