

Gradient Flows — Exercises

Exercise 1 (φ -divergences and Wasserstein gradient flow). Let ν be a reference probability measure on \mathbb{R}^d and let $\varphi : \mathbb{R}_+ \rightarrow \mathbb{R}$ be a convex \mathcal{C}^1 function with $\varphi(1) = 0$. For a probability measure α such that $\alpha \ll \nu$ with density $\rho := \frac{d\alpha}{d\nu}$, the φ -divergence of α with respect to ν is defined by

$$D_\varphi(\alpha \mid \nu) := \int_{\mathbb{R}^d} \varphi\left(\frac{d\alpha}{d\nu}(x)\right) d\nu(x) = \int_{\mathbb{R}^d} \varphi(\rho(x)) d\nu(x).$$

- (1) Show that $D_\varphi(\alpha \mid \nu) \geq 0$.
- (2) Consider the functional $f(\alpha) := D_\varphi(\alpha \mid \nu)$ on $\mathcal{W}_2(\mathbb{R}^d)$. Assume that both ν and α admit smooth strictly positive densities with respect to Lebesgue measure.
 - (a) Compute the first variation $\frac{\delta f}{\delta \alpha}(\alpha)(x)$ and deduce the Wasserstein gradient $\nabla_{\mathcal{W}} f(\alpha)(x)$.
 - (b) Write the corresponding Wasserstein gradient flow PDE.
 - (c) Specialize your formulas to the case $\varphi(s) = s \log s$.

Exercise 2 (Gradient flows of Dirichlet energy and Fisher information). We denote α_t be a family of probability measures on \mathbb{R}^d with smooth positive density $\alpha_t(dx) = \rho_t(x) dx$.

- (1) Consider the Dirichlet energy $\mathcal{E}(\alpha) := \int_{\mathbb{R}^d} |\nabla \rho(x)|^2 dx$, $\rho = \frac{d\alpha}{dx}$.
 - (a) Compute first variation $\delta f(\alpha)$ and write down the “ $L^2(dx)$ ” gradient flow PDE, which is $\partial_t \rho_t = \delta f(\alpha_t)$ ie. the steepest descent for \mathcal{E} with respect to the $L^2(dx)$ metric.
 - (b) Compute the \mathcal{W}_2 -gradient of \mathcal{E} and write the associated Wasserstein gradient flow PDE.
- (2) Consider now the Fisher information $\mathcal{I}(\alpha) := \int_{\mathbb{R}^d} |\nabla \log \rho(x)|^2 dx$, $\rho = \frac{d\alpha}{dx}$. Same questions.

Exercise 3 (Gaussian evolution under linear dynamics). Let $(X_t)_{t \in \mathbb{N}}$ be a sequence of random variables in \mathbb{R}^d defined by the linear recursion

$$X_{t+1} = X_t - \tau A_t X_t, \quad t = 0, 1, 2, \dots,$$

where $\tau > 0$ is a fixed step size and, for each t , $A_t \in \mathbb{R}^{d \times d}$ is a deterministic matrix. Denote by α_t the law of X_t .

- (1) Assume that the initial condition is Gaussian $X_0 \sim \mathcal{N}(0, \Sigma_0)$, for some symmetric positive semidefinite covariance matrix $\Sigma_0 \in \mathbb{R}^{d \times d}$. Show that each X_t is also Gaussian, and describe the evolution of the law $\alpha_t = \mathcal{L}(X_t)$ by giving an explicit recursion for the covariance matrices Σ_t .
- (2) Consider now the continuous time ODE $\dot{X}_t = -A_t X_t$, $t \geq 0$, with $A_t \in \mathbb{R}^{d \times d}$ a (say, continuous) time dependent matrix and random initial condition $X_0 \sim \mathcal{N}(0, \Sigma_0)$. Explain why X_t is Gaussian for every $t \geq 0$, say $X_t \sim \mathcal{N}(0, \Sigma_t)$, and, by considering the limit $\tau \rightarrow 0$ in the discrete time recursion from part (1), show that $(\Sigma_t)_{t \geq 0}$ solves a matrix ODE that you should identify.

Exercise 4 (Wasserstein flow for quadratic kernels). Let $\alpha \in \mathcal{P}_2(\mathbb{R}^d)$ and denote its mean and covariance by

$$m(\alpha) := \int_{\mathbb{R}^d} x d\alpha(x), \quad \Sigma(\alpha) := \int_{\mathbb{R}^d} (x - m(\alpha))(x - m(\alpha))^\top d\alpha(x).$$

Consider the functionals

$$f(\alpha) := \iint_{\mathbb{R}^d \times \mathbb{R}^d} k(x, y) d\alpha(x) d\alpha(y)$$

on the Wasserstein space $\mathcal{W}_2(\mathbb{R}^d)$, where the kernels k are given below.

- (1) Let $k(x, y) = \langle Ax, y \rangle$, $A \in \mathbb{R}^{d \times d}$.
- (a) Express $f(\alpha)$ in terms of $m(\alpha)$ and A .
 - (b) Compute the Wasserstein gradient $\nabla_W f(\alpha)$.
 - (c) Write the Wasserstein gradient flow PDE, and, for a general initial condition $\alpha_{t=0} = \alpha_0$, give an explicit expression of α_t in terms of α_0 .
- (2) Let $k(x, y) = \langle Ax, y \rangle \langle Bx, y \rangle$, $A, B \in \mathbb{R}^{d \times d}$.
- (a) Compute the Wasserstein gradient $\nabla_W f(\alpha)$.
 - (b) Using the previous exercise on linear ODEs with Gaussian initial data, show that if $\alpha_{t=0} = \mathcal{N}(0, \Sigma_0)$, then $\alpha_t = \mathcal{N}(0, \Sigma_t)$ for all $t \geq 0$, and derive the matrix ODE satisfied by $(\Sigma_t)_{t \geq 0}$.

Optional – More difficult exercises

Exercise 5 (Mean-field two-layer linear network under Wasserstein flow). Let ρ be a probability measure on \mathbb{R}^d (the data distribution) and $h : \mathbb{R}^d \rightarrow \mathbb{R}$ a target function. For a parameter distribution

$$\alpha \in \mathcal{P}_2(\mathbb{R} \times \mathbb{R}^d), \quad x = (u, v) \in \mathbb{R} \times \mathbb{R}^d,$$

consider the two-layer linear mean-field model

$$g_\alpha(z) := \int u \langle z, v \rangle d\alpha(u, v), \quad z \in \mathbb{R}^d,$$

and the quadratic loss

$$f(\alpha) := \int_{\mathbb{R}^d} |g_\alpha(z) - h(z)|^2 d\rho(z).$$

(1) Show that f can be written as a quadratic functional of α of the form

$$f(\alpha) = \iint k(x, y) d\alpha(x) d\alpha(y) + \int b(x) d\alpha(x) + c,$$

where $x = (u, v)$, $y = (u', v')$, and identify explicit formulas for $k(x, y)$ and $b(x)$ in terms of ρ and h . You may leave the constant c implicit.

(2) Consider the Wasserstein gradient flow of f on $\mathcal{W}_2(\mathbb{R} \times \mathbb{R}^d)$:

$$\partial_t \alpha_t + \nabla \cdot (\alpha_t v_t) = 0, \quad v_t(x) = -\nabla_W f(\alpha_t)(x).$$

Using the structure from part (1) and the previous exercise on quadratic kernels, show that if

$$\alpha_{t=0} = \mathcal{N}(0, \Sigma_0),$$

then α_t remains Gaussian for all $t \geq 0$.

Solution. (1) **Quadratic representation of the loss.**

Write $x = (u, v)$ and $y = (u', v')$, with $u, u' \in \mathbb{R}$ and $v, v' \in \mathbb{R}^d$. The model output can be written as

$$g_\alpha(z) = \int u \langle z, v \rangle d\alpha(u, v) = \int \phi_x(z) d\alpha(x), \quad \phi_x(z) := u \langle z, v \rangle.$$

Then

$$f(\alpha) = \int (g_\alpha(z) - h(z))^2 d\rho(z) = \int g_\alpha(z)^2 d\rho(z) - 2 \int g_\alpha(z) h(z) d\rho(z) + \int h(z)^2 d\rho(z).$$

The last term does not depend on α , so it can be absorbed into a constant c .

For the quadratic term,

$$\begin{aligned} \int g_\alpha(z)^2 d\rho(z) &= \int \left(\int \phi_x(z) d\alpha(x) \right)^2 d\rho(z) \\ &= \int \left(\int \phi_x(z) d\alpha(x) \right) \left(\int \phi_y(z) d\alpha(y) \right) d\rho(z) \\ &= \iint \left(\int \phi_x(z) \phi_y(z) d\rho(z) \right) d\alpha(x) d\alpha(y). \end{aligned}$$

This suggests the kernel

$$k(x, y) := \int \phi_x(z) \phi_y(z) d\rho(z) = \int u u' \langle z, v \rangle \langle z, v' \rangle d\rho(z).$$

It is convenient to express this in terms of the covariance of ρ :

$$K := \int z z^\top d\rho(z) \in \mathbb{R}^{d \times d}.$$

Then

$$\int \langle z, v \rangle \langle z, v' \rangle d\rho(z) = v^\top \left(\int z z^\top d\rho(z) \right) v' = v^\top K v'.$$

Hence

$$k(x, y) = u u' v^\top K v'.$$

For the linear term,

$$\begin{aligned} -2 \int g_\alpha(z) h(z) d\rho(z) &= -2 \int \left(\int \phi_x(z) d\alpha(x) \right) h(z) d\rho(z) \\ &= -2 \int \left(\int \phi_x(z) h(z) d\rho(z) \right) d\alpha(x), \end{aligned}$$

so we can write

$$b(x) := -2 \int \phi_x(z) h(z) d\rho(z) = -2u \int \langle z, v \rangle h(z) d\rho(z).$$

Define

$$c_h := \int z h(z) d\rho(z) \in \mathbb{R}^d,$$

so that

$$\int \langle z, v \rangle h(z) d\rho(z) = \langle v, c_h \rangle.$$

Then

$$b(x) = -2u \langle v, c_h \rangle.$$

Putting these pieces together,

$$f(\alpha) = \iint k(x, y) d\alpha(x) d\alpha(y) + \int b(x) d\alpha(x) + c,$$

with

$$k(x, y) = u u' v^\top K v', \quad b(x) = -2u \langle v, c_h \rangle,$$

and $c = \int h(z)^2 d\rho(z)$.

(2) Gaussian preservation under Wasserstein flow.

We now consider the Wasserstein gradient flow of f :

$$\partial_t \alpha_t + \nabla \cdot (\alpha_t v_t) = 0, \quad v_t(x) = -\nabla_W f(\alpha_t)(x).$$

First variation and gradient structure. From the representation

$$f(\alpha) = \iint k(x, y) d\alpha(x) d\alpha(y) + \int b(x) d\alpha(x) + c,$$

with a symmetric kernel k , the first variation can be written as

$$\frac{\delta f}{\delta \alpha}(\alpha)(x) = 2 \int k(x, y) d\alpha(y) + b(x) + \text{const.}$$

Therefore the Wasserstein gradient is

$$\nabla_W f(\alpha)(x) = \nabla_x \left(2 \int k(x, y) d\alpha(y) + b(x) \right).$$

Using the explicit formulas for k and b , we see that for fixed α the map

$$x \mapsto 2 \int k(x, y) d\alpha(y) + b(x)$$

is a polynomial of degree at most two in the coordinates of $x = (u, v)$. Indeed:

- $k(x, y)$ is bilinear in x and y , so integrating in y leaves a function that is quadratic in x .
- $b(x)$ is bilinear in (u, v) , so it is also quadratic in x .

As a consequence, its gradient with respect to x is *linear* in x :

$$\nabla_W f(\alpha)(x) = M(\alpha)x + \ell(\alpha),$$

for some matrix $M(\alpha)$ and vector $\ell(\alpha)$ that depend on α only through its low order moments (essentially mean and covariance).

Hence the velocity field in the gradient flow has the affine form

$$v_t(x) = -\nabla_W f(\alpha_t)(x) = -M_t x - \ell_t,$$

where we write $M_t := M(\alpha_t)$ and $\ell_t := \ell(\alpha_t)$.

Reduction to linear ODEs. A Wasserstein gradient flow with velocity field of the form

$$v_t(x) = -M_t x - \ell_t$$

corresponds to a nonlinear (in law) dynamics for a random parameter $X_t = (U_t, V_t)$:

$$\dot{X}_t = -M_t X_t - \ell_t,$$

in the sense that $\alpha_t = \mathcal{L}(X_t)$ is a weak solution of the continuity equation. Here M_t and ℓ_t are deterministic functions of the current law α_t , but for each fixed t the dynamics in x are linear and homogeneous plus a translation.

Consider an initial condition

$$\alpha_0 = \mathcal{N}(0, \Sigma_0),$$

so that X_0 is Gaussian with mean zero and covariance Σ_0 . The previous exercise established that linear ODEs of the form

$$\dot{X}_t = -A_t X_t \quad \text{or more generally} \quad \dot{X}_t = -A_t X_t - b_t,$$

with deterministic A_t and b_t , preserve Gaussianity of the law: if X_0 is Gaussian, then X_t is Gaussian for all t , and the mean and covariance solve closed ODEs.

In our setting, at each time t the right-hand side is linear in X_t plus a constant vector:

$$\dot{X}_t = -M_t X_t - \ell_t.$$

Conditionally on the path $(M_s, \ell_s)_{s \leq t}$, this is a linear deterministic ODE in X_t . Therefore, starting from a Gaussian X_0 , the solution X_t remains Gaussian for every $t \geq 0$.

Equivalently, the law $\alpha_t = \mathcal{L}(X_t)$ stays in the family of Gaussian measures:

$$\alpha_t = \mathcal{N}(m_t, \Sigma_t),$$

with (m_t, Σ_t) following a closed system of ODEs derived by applying the linear ODE covariance computation from the previous exercise. In particular, if $m_0 = 0$, then m_t stays zero and only the covariance evolves.

Conclusion. Since the Wasserstein gradient of f is affine linear in the parameter x , the associated Wasserstein gradient flow acts on parameters through a linear ODE with time dependent coefficients. By the result on linear dynamics with Gaussian initial data, this implies that if

$$\alpha_{t=0} = \mathcal{N}(0, \Sigma_0),$$

then α_t is Gaussian for every $t \geq 0$.

Exercise 6 (Wasserstein flow of W_2^2). Fix $\beta \in \mathcal{P}_2(\mathbb{R}^d)$. For $\alpha \in \mathcal{P}_2(\mathbb{R}^d)$ define $f(\alpha) := W_2(\alpha, \beta)^2$. Assume α has a smooth strictly positive density and consider the quadratic cost $c(x, y) = \frac{1}{2}|x - y|^2$.

- (1) Using the Kantorovich dual problem, and using the envelope theorem (that was used the same way in the previous exercise sheet for discrete measure), compute the first variation $\delta f(\alpha)$.
- (2) Assume α is absolutely continuous. Leveraging Brenier's theorem connecting the transport map T to the dual potential, compute the Wasserstein gradient $\nabla_W f(\alpha)$.
- (3) Relate the Wasserstein flow $(\alpha_t)_{t \geq 0}$ to the McCann interpolation (you should use Benamou-Brenier dynamical formulation which details a valid field advecting the interpolant).

Solution. Throughout we work with the quadratic cost $c(x, y) = \frac{1}{2}|x - y|^2$ so that $F(\alpha) := \frac{1}{2}W_2(\alpha, \beta)^2$ has a clean Kantorovich dual representation.

(1) Dual formulation and envelope theorem.

The Kantorovich dual problem for $F(\alpha) = \frac{1}{2}W_2(\alpha, \beta)^2$ reads

$$F(\alpha) = \sup_{\varphi, \psi} \left\{ \int \varphi d\alpha + \int \psi d\beta : \varphi(x) + \psi(y) \leq \frac{1}{2}|x - y|^2 \quad \forall x, y \right\}.$$

For the moment fix β and view F as a functional of α . For each admissible pair (φ, ψ) , define

$$\mathcal{J}(\alpha; \varphi, \psi) := \int \varphi d\alpha + \int \psi d\beta.$$

Then

$$F(\alpha) = \sup_{(\varphi, \psi) \in \mathcal{A}} \mathcal{J}(\alpha; \varphi, \psi),$$

where \mathcal{A} is the set of admissible potentials. Suppose that for the given α there exists an optimal pair $(\varphi_\alpha, \psi_\alpha) \in \mathcal{A}$ such that

$$F(\alpha) = \mathcal{J}(\alpha; \varphi_\alpha, \psi_\alpha),$$

and that this pair is unique up to an additive constant (this holds under mild conditions).

Formally, one can apply an infinite-dimensional variant of the envelope theorem: the derivative of a supremum with respect to a parameter is obtained by differentiating the objective at an optimal argument, ignoring the derivative of the optimizer itself. Concretely, let σ be a signed measure with zero total mass and consider a perturbation $\alpha_\varepsilon = \alpha + \varepsilon\sigma$ (for small ε and in a formal sense). Then

$$F(\alpha_\varepsilon) = \sup_{(\varphi, \psi) \in \mathcal{A}} \mathcal{J}(\alpha_\varepsilon; \varphi, \psi) \geq \mathcal{J}(\alpha_\varepsilon; \varphi_\alpha, \psi_\alpha) = \int \varphi_\alpha d\alpha_\varepsilon + \int \psi_\alpha d\beta.$$

On the other hand, optimality of $(\varphi_\alpha, \psi_\alpha)$ at α ensures that

$$F(\alpha) = \mathcal{J}(\alpha; \varphi_\alpha, \psi_\alpha) \geq \mathcal{J}(\alpha; \varphi, \psi) \quad \text{for all } (\varphi, \psi) \in \mathcal{A}.$$

Assuming enough regularity and differentiability so that the envelope theorem applies, the directional derivative of F at α in direction σ is obtained by differentiating \mathcal{J} at the optimal pair:

$$\left. \frac{d}{d\varepsilon} F(\alpha_\varepsilon) \right|_{\varepsilon=0} = \left. \frac{d}{d\varepsilon} \mathcal{J}(\alpha_\varepsilon; \varphi_\alpha, \psi_\alpha) \right|_{\varepsilon=0} = \int \varphi_\alpha d\sigma.$$

By definition of the first variation, this means

$$\frac{\delta F}{\delta \alpha}(\alpha)(x) = \varphi_\alpha(x) + \text{const.}$$

Since $f(\alpha) = W_2(\alpha, \beta)^2 = 2F(\alpha)$, we obtain

$$\frac{\delta f}{\delta \alpha}(\alpha)(x) = 2\varphi_\alpha(x) + \text{const.}$$

The additive constant is irrelevant for the Wasserstein gradient.

(2) Link to Brenier map and identification of $\nabla_W f$.

Assume now that α has a density with respect to Lebesgue measure. By Brenier's theorem, there exists a convex function $u_\alpha : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$T_\alpha(x) := \nabla u_\alpha(x)$$

is the unique optimal transport map from α to β for the cost $c(x, y) = \frac{1}{2}|x - y|^2$, and

$$(T_\alpha)_\# \alpha = \beta, \quad \frac{1}{2}W_2(\alpha, \beta)^2 = \int \frac{1}{2}|x - T_\alpha(x)|^2 d\alpha(x).$$

For the quadratic cost, any optimal potential φ_α can be written as

$$\varphi_\alpha(x) = \frac{1}{2}|x|^2 - u_\alpha(x) + c_\alpha,$$

for some constant c_α . This comes from the c -transform representation: the c -transform of a convex function u with cost $\frac{1}{2}|x - y|^2$ is

$$\varphi(x) = \inf_y \left\{ \frac{1}{2}|x - y|^2 - \psi(y) \right\} = \frac{1}{2}|x|^2 - u(x),$$

with u convex. For an optimal pair, u coincides with the Brenier potential u_α .

Differentiating the expression for φ_α gives

$$\nabla \varphi_\alpha(x) = x - \nabla u_\alpha(x) = x - T_\alpha(x).$$

From the first variation above,

$$\frac{\delta f}{\delta \alpha}(\alpha)(x) = 2\varphi_\alpha(x) + \text{const},$$

so the Wasserstein gradient (in Otto's formal Riemannian calculus) is the spatial gradient of the first variation:

$$\nabla_W f(\alpha)(x) = \nabla_x \left(\frac{\delta f}{\delta \alpha}(\alpha)(x) \right) = 2 \nabla \varphi_\alpha(x) = 2(x - T_\alpha(x)).$$

This recovers, in a more systematic way, the informal formula used earlier.

(3) Wasserstein flow and McCann interpolation.

The Wasserstein gradient flow of f is defined by

$$\partial_t \alpha_t + \nabla \cdot (\alpha_t v_t) = 0, \quad v_t(x) = -\nabla_W f(\alpha_t)(x).$$

Using the expression from the previous item, if T_t denotes the optimal transport map from α_t to β , we have

$$v_t(x) = -2(x - T_t(x)) = 2(T_t(x) - x).$$

So the PDE for the density ρ_t of α_t is

$$\partial_t \rho_t + \nabla \cdot (\rho_t 2(T_t - \text{Id})) = 0, \quad (T_t)_\# \alpha_t = \beta.$$

Now let us connect this with the McCann interpolation between α_0 and β . Let T be the optimal transport map from α_0 to β (for the same cost). McCann's displacement interpolation defines a constant-speed geodesic $(\mu_s)_{s \in [0,1]}$ in (\mathcal{P}_2, W_2) by

$$\mu_s = ((1 - s)\text{Id} + sT)_\# \alpha_0.$$

One can check that

$$W_2(\mu_s, \beta) = (1 - s) W_2(\alpha_0, \beta).$$

Formally, Wasserstein space behaves like a Riemannian manifold, and the tangent vector to the geodesic (μ_s) at time s is represented by the velocity field

$$w_s(x) = T_s(x) - x,$$

where T_s is the optimal map from μ_s to β . Along this geodesic, the gradient of $f(\cdot) = W_2(\cdot, \beta)^2$ at μ_s points in the direction of $x - T_s(x)$, that is opposite to the direction w_s . More precisely, from the computation above

$$\nabla_W f(\mu_s)(x) = 2(x - T_s(x)) = -2 w_s(x),$$

and the negative gradient (the direction of steepest decrease) is

$$-\nabla_W f(\mu_s)(x) = 2 w_s(x),$$

which is exactly the geodesic velocity scaled by a factor 2.

This is completely analogous to the finite dimensional situation on a Riemannian manifold with metric distance d : the gradient of the function $p \mapsto \frac{1}{2}d(p, q)^2$ at a point on the geodesic from p_0 to q is a multiple of the geodesic velocity vector. As a consequence, the gradient flow of $d(\cdot, q)^2$ follows the geodesic to q , but with a nonlinear time parametrization (exponential in time rather than linear).

Translating this heuristic picture to Wasserstein space:

- Fix the geodesic $(\mu_s)_{s \in [0,1]}$ from α_0 to β given by McCann's interpolation.
- Its initial velocity at $s = 0$ is $w_0(x) = T(x) - x$.
- The Wasserstein gradient at α_0 is $\nabla_W f(\alpha_0)(x) = 2(x - T(x)) = -2w_0(x)$, so the gradient flow starting at α_0 moves in the same direction as the McCann geodesic, only faster by a factor 2 in this tangent sense.

With a bit more formal Otto calculus, one can show that the trajectory $(\alpha_t)_{t \geq 0}$ of the gradient flow can be written as

$$\alpha_t = \mu_{s(t)}, \quad s(0) = 0,$$

where $s(t) \in [0, 1)$ solves a scalar ODE of the type

$$\dot{s}(t) = 2(1 - s(t)),$$

so that $s(t) = 1 - e^{-2t}$. In other words, the gradient flow follows the McCann interpolation, but reparametrized in time so that it reaches β only in the infinite time limit and with an exponential rate of convergence in W_2 :

$$W_2(\alpha_t, \beta) = (1 - s(t)) W_2(\alpha_0, \beta) = e^{-2t} W_2(\alpha_0, \beta).$$