Gradient flows and PDEs

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April 17, 2024

Outline

• Goals:

- ▶ What are gradient flows (GF) on the space of probability measures?
- How are GFs connected to PDEs?
- Why is this useful?

• Part I:

- GF on \mathbb{R}^d .
- GF on space of probability measures.
- Connection to PDEs.
- Following: [AGS] "Gradient Flows in Metric Spaces and in the Space of Probability Measures" by Ambrosio, Gigli, Savaré.

Part II:

- Recent work on particle methods for nonlinear diffusion equations.
- ▶ Joint work with K. Craig, K. Elamvazhuthi, M. Haberland (2022).

Part I

Gradient flows on Euclidean space

• Let
$$F : \mathbb{R}^d \to (-\infty, +\infty]$$
 be λ -convex, some $\lambda \in \mathbb{R}$.

• This means $F(x) - \frac{\lambda}{2}|x|^2$ is convex.

• Let $x_0 \in \mathbb{R}^d$. Gradient flow of F on \mathbb{R}^d is a curve $x : [0, T] \to \mathbb{R}^d$ such that

$$\begin{cases} x'(t) &= -\nabla F(x(t)) \text{ for } t > 0, \\ x(0) &= x_0. \end{cases}$$
 (ODE)

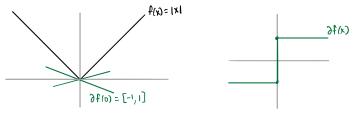
• F is λ -convex $\implies \nabla F$ is Lipschitz \implies ODE has a solution for all $x_0 \in \mathbb{R}^d$.

Subdifferential of λ -convex $F : \mathbb{R}^d \to (-\infty, +\infty]$

• We say $p \in \mathbb{R}^d$ is in the subdifferential of F at x, denoted $p \in \partial F(x)$, if

$$\mathsf{F}(y)-\mathsf{F}(x)\geq (y-x)\cdot \mathsf{p}+rac{\lambda}{2}|x-y|^2 ext{ for all } y\in \mathbb{R}^d.$$

- If x s.t. F is differentiable at x, then $\partial F(x) = \{\nabla F(x)\}.$
- Example ($\lambda = 0$):



• Reformulate (ODE) as,

$$\begin{cases} x'(t) \in -\partial F(x(t)) & \text{for } t > 0, \\ x(0) &= x_0. \end{cases}$$

GF on $\mathcal{P}_2(\mathbb{R}^d)$?

• On Euclidean space: $F \lambda$ -convex,

$$egin{cases} x'(t) &\in -\partial F(x(t)) \quad ext{for } t>0, \ x(0) &= x_0. \end{cases}$$

- $\mathcal{P}_2(\mathbb{R}^d)$ (probability measures with finite second moment) equipped with W_2 distance.
- For $\mu \ll dx$, we denote its density by μ as well.
- Energies $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ that are proper, lower semicontinous wrt W_2 , and λ -convex.
- Let $\mathcal{F}: \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ be proper, lower semicontinous wrt W_2 , and λ -convex.
- To formulate analogous definition in $\mathcal{P}_2(\mathbb{R}^d)$, need notions of:
 - A curve $\mu(t)$ and its time derivative,
 - Subdifferential of *F*.

Time derivative of a curve $\mu : [0, T] \to \mathcal{P}_2(\mathbb{R}^d)$

• Definition: metric derivative

$$|\mu'|(t):=\lim_{s
ightarrow t}rac{W_2(\mu(t),\mu(s))}{|t-s|}$$

- We consider curves µ ∈ AC²([0, T]; P₂(ℝ^d)); for such curves this limit is well-defined.
- We use $\mu(t)$ to denote $\mu(\cdot, t)$.
- $|\mu'|(t) \in \mathbb{R}$; not quite analogous to $x'(t) \in \mathbb{R}^d$.
- Theorem [AGS 8.3.1]: $|\mu'|(t)$ is the metric derivative of μ "if and only if"

$$\partial_t \mu +
abla \cdot (oldsymbol{v}\mu) = 0$$
 weakly on $[0, T] imes \mathbb{R}^d$

holds for a velocity field $\boldsymbol{v}:[0,T] \times \mathbb{R}^d \to \mathbb{R}^d$, $\boldsymbol{v}(t,\cdot) \in L^2(\mu(t);\mathbb{R}^d)$, with

$$|\mu'(t)| = \|\mathbf{v}\|_{L^2(\mu(t);\mathbb{R}^d)}$$
 a.e. t.

• \mathbf{v} will be our analogy of x'.

Subdifferential of λ -convex \mathcal{F}

Definition: Let μ ∈ D(F). We say ξ : ℝ^d → ℝ^d with ξ ∈ L²(μ; ℝ^d) is in the subdifferential of F at μ if for all ν ∈ P₂(ℝ^d),

$$\mathcal{F}(
u) - \mathcal{F}(\mu) \geq \int_{\mathbb{R}^d imes \mathbb{R}^d} \langle \boldsymbol{\xi}(x), y - x
angle d oldsymbol{\gamma}(x, y) + rac{\lambda}{2} W_2^2(\mu,
u)$$

for all $\gamma \in \Gamma_0(\mu, \nu)$. We write $\boldsymbol{\xi} \in \partial \mathcal{F}(\mu)$.

• Attempt 1: Let $\mathbf{v} \in L^2(\mu; \mathbb{R}^d)$ be "time derivate of μ " as on previous slide. How about

$$\mathbf{v}(t) \in -\partial \mathcal{F}(\mu(t))?$$

- Not quite: there could be tons of stuff in the subdifferential.
- Theorem [AGS 10.1.5]: For "nice" μ ∈ P₂(ℝ^d), the subdifferential ∂F(μ) has an element of minimal norm (|| · ||_{L²(μ:ℝ^d)}). This element is denoted ∂°F(μ).

$\mathsf{GF} \text{ of } \lambda \text{-convex } \mathcal{F}$

Definition [AGS 11.1.1]: We say μ ∈ AC²([0, T], P₂(ℝ^d)) is a gradient flow of F if μ(t) solves

$$\partial_t \mu + \nabla \cdot (\mathbf{v}\mu) = 0, \tag{1}$$

and,

$$\mathbf{v}(t) = -\partial^{\circ} \mathcal{F}(\mu(t))$$
 a.e. $t \in [0, T]$.

- Theorem [AGS 11.2.1]: Suppose $\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to (-\infty, +\infty]$ is proper, lsc, and λ -convex, and $\mu^0 \in \overline{D(\mathcal{F})}$. Then, there exists a unique gradient flow $\mu(t)$ of \mathcal{F} with initial condition μ^0 .
- The continuity equation (1) will connect GF to PDEs, once we characterize −∂°F(µ(t)) explicitly.

$\partial^{\circ}\mathcal{F}(\mu)$ and PDEs

• Formally (for twice differentiable μ , nice \mathcal{F}):

$$\mathcal{F}(\mu) = \int F(x,\mu(x),\nabla\mu(x)) \, dx \implies \partial^{\circ} \mathcal{F}(\mu) = \nabla \frac{\delta \mathcal{F}}{\delta \mu},$$

where $\frac{\delta \mathcal{F}}{\delta x}$ is the first variation of \mathcal{F} .

• More generally: V convex, W convex and even, f convex (and more):

$$\begin{array}{c|cc}
\mathcal{F} & \partial^{\circ}\mathcal{F}(\mu) & \mathsf{PDE} \\
\hline \mathcal{V}(\mu) = \int V(x) \, d\mu & \nabla V & \partial_t \mu - \operatorname{div}(\mu \nabla V) = 0 \\
\hline \mathcal{W}(\mu) = \int W(x - y) d\mu(x) d\mu(y) & \nabla W * \mu & \partial_t \mu - \operatorname{div}(\mu \nabla W * \mu) = 0 \\
\hline \mathcal{E}(\mu) = \int f(\mu) \, dx & \nabla f'(\mu) & \partial_t \mu - \nabla(\mu \nabla f'(\mu)) = 0 \\
\end{array}$$

• Subexamples:

- $f(s) = s \log s s \iff$ heat equation.
- $f(s) = \frac{1}{m-1}s^m \iff$ porous medium eq'n (m > 1), fast diffusion $(\frac{d}{d+2} < m < 1)$.
- $\mathcal{F} := \mathcal{E} + \mathcal{V} + \mathcal{W}$, say, yields corresponding drift-diffusion-aggregation PDE.

Curve of maximal slope: Euclidean space

• Let y(t) be any curve.

$$F(y(0)) - F(y(t)) = \int_0^t -\frac{d}{dr} F(y(r)) \, dr = \int_0^t -\nabla F(y(r)) y'(r) \, dr$$

$$\leq \frac{1}{2} \int_0^t |\nabla F(y(r))|^2 \, dr + \frac{1}{2} \int_0^t |y'(r)|^2 \, dr,$$

with equality holding $\iff y'(r) = -\nabla F(y(r))$ for a.e. r. • So x(t) is GF of $F \iff$ equality holds $\iff \ge$ holds \iff

$$F(x(0)) - F(x(t)) \geq \frac{1}{2} \int_0^t \int_0^t |\nabla F(x(r))|^2 dr + \frac{1}{2} \int_0^t |x'(r)|^2 dr.$$

Theorem [AGS 11.2.1]: For "nice" *F*, μ is the gradient flow of *F* ⇔ μ is a *Curve of Maximal Slope*; i.e., for all t ∈ [0, T],

$$\mathcal{F}(\mu(0)) - \mathcal{F}(\mu(t)) \geq rac{1}{2} \int_0^t |\partial \mathcal{F}|^2(\mu(r)) dr + rac{1}{2} \int_0^t |\mu'|^2(r) dr.$$

- Here $|\partial \mathcal{F}|(\mu(r))$ is the metric slope of \mathcal{F} at $\mu(r)$.
- We can think $|\partial \mathcal{F}|(\mu) = ||\partial^{\circ} \mathcal{F}(\mu)||_{L^{2}(\mu;\mathbb{R}^{d})}$.

JKO (Jordan-Kinderleher-Otto) scheme

$$x'(t) = -\nabla F(x), \quad x(0) = x_0.$$

• Fix small time step $\tau > 0$, let $x_0^{\tau} = x_0$, and define, for $k \ge 1$,

$$x_{k+1}^{ au} = \operatorname{argmin}\left(F(x) + \frac{|x - x_k^{ au}|^2}{2 au}
ight),$$

which implies $-\nabla F(x_{k+1}^{\tau}) = \frac{x_{k+1}^{\tau} - x_k^{\tau}}{\tau}$ holds.

- The x_k^{τ} converge to x(t) as $\tau \to 0$ (implicit Euler scheme.)
- "JKO scheme" for \mathcal{F} : given initial data μ_0 , define, for $k \geq 1$,

$$\mu_{k+1}^{ au} = \operatorname{argmin}\left(\mathcal{F}(\mu) + \frac{W_2(\mu, \mu_k^{ au})^2}{2 au}
ight).$$

Theorem [AGS 11.2.1]: For "nice" *F*, there exists a limiting μ, and it's a GF of *F* in the previous sense.

Remark

- We've seen three equivalent (for "nice" \mathcal{F}) formulations of GFs on $\mathcal{P}_2(\mathbb{R}^d)$:
 - Pointwise-differential formulation
 - Curve of maximal slope
 - Minimizing movement scheme.
- There are others!

Part II

Introduction

- Fix $\Omega \subset \mathbb{R}^d$ (convex) and $\bar{\rho} : \Omega \to \mathbb{R}^+$ (log-concave), nice.
- We focus on:

$$\begin{cases} \partial_t \rho - \operatorname{div}\left(\rho \nabla\left(\frac{\rho}{\overline{\rho}}\right)\right) = 0 \text{ in } \Omega \times (0, \infty), \\ \partial_\nu \left(\frac{\rho}{\overline{\rho}}\right) = 0 \text{ on } (\partial\Omega) \times (0, \infty). \end{cases}$$
(D)

• If $ar{
ho}\equiv$ 1, then the diffusion term becomes,

$$\operatorname{div}(\rho \nabla \rho) = rac{1}{2} \operatorname{div}(\nabla \rho^2) = rac{1}{2} \Delta(\rho^2).$$

So this PDE is an inhomogeneous porous medium equation.

• Today: deterministic particle method.

• Challenge:
$$\rho(0) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_i^0} \Rightarrow \rho(t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_i(t)}$$
.

Introduction

• Part I stuff implies:

$$\partial_t \rho - \operatorname{div}\left(\rho \nabla\left(\frac{\rho}{\bar{\rho}}\right)\right) = 0 \quad \iff \quad \rho \text{ GF of } \mathcal{E}[\rho] = \frac{1}{2} \int \frac{\rho}{\bar{\rho}} \, d\rho.$$

• Main idea:

$\mathsf{regularize}\ \mathcal{E}$

in a way that ensures "particles remain particles."

• We define the regularized energy

$$\mathcal{E}_{\varepsilon}[\rho] = rac{1}{2} \int rac{(
ho * \zeta_{\varepsilon})^2}{\overline{
ho}} \, dx,$$

where ζ_{ε} is a mollifier "with enough decay."

- This idea originates from Lions, Mas-Gallic (2001): study PME, $\bar{\rho} \equiv 1$.
- Carillo, Craig, Patacchini (2019): $\bar{\rho} \equiv 1$ and with aggregation and drift.
- Related work: Oelschlöger (1990); Lu, Slepčev, Wang (2023); Carrillo, Esposito, Wu (2023); Craig, Jacobs, T. (2023).

On the convex domain $\Omega \subset \mathbb{R}^d$

$$\begin{cases} \partial_t \rho - \operatorname{div}\left(\rho \nabla\left(\frac{\rho}{\bar{\rho}}\right)\right) = 0 \text{ in } \Omega \times (0,\infty), \\ \partial_\nu\left(\frac{\rho}{\bar{\rho}}\right) = 0 \text{ on } (\partial\Omega) \times (0,\infty). \end{cases}$$
(D)

• Solutions to (D) are Wasserstein gradient flows of the energy:

$$\mathcal{F}[\rho] = \mathcal{E}[\rho] + \mathcal{V}_{\Omega}[\rho], \quad \text{ where } \ \mathcal{V}_{\Omega}[\rho] = \begin{cases} 0 \text{ if } \operatorname{supp} \rho \subset \bar{\Omega}, \\ +\infty \text{ otherwise.} \end{cases}$$

• We also approximate \mathcal{V}_Ω via a "soft cutoff potential":

$$\mathcal{V}_k[
ho] := \int_{\mathbb{R}^d} V_k \, d
ho, \quad ext{ where } egin{cases} V_k(x) = 0 & ext{ for all } x \in ar{\Omega}, ext{ for all } k, \ V_k(x) o +\infty & ext{ as } k o \infty ext{ for } x \in ar{\Omega}^c. \end{cases}$$

• Main result: take $\varepsilon \to 0$ and $k \to \infty$ in

$$\mathcal{F}_{\varepsilon,k} = \mathcal{E}_{\varepsilon} + \mathcal{V}_k.$$

The approximation and particle data

Lemma: GFs of $\mathcal{F}_{\varepsilon,k}$ are well-defined and are distributional solutions of

$$\partial_t \rho - \operatorname{div}\left(\rho \nabla \left(\zeta_{\varepsilon} * \left(\frac{\zeta_{\varepsilon} * \rho}{\overline{\rho}}\right) + V_k\right)\right) = 0.$$

Lemma: Let $\rho_{\varepsilon,k}^N$ denote the GF of $\mathcal{F}_{\varepsilon,k}$ with initial data $\frac{1}{N} \sum_{i=1}^N \delta_{X_i^0}$. We have, for t > 0,

$$\rho_{\varepsilon,k}^{N}(x,t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_{i}(t)},$$

. .

where the X_i evolve via the system of ODEs associated to the continuity equation:

$$rac{d}{dt}X_{j}(t)=-V_{arepsilon}^{(j)}(X_{1}(t),...,X_{N}(t)), \quad X_{j}(0)=X_{j}^{0},$$

where V_{ε} is given by,

$$V_{\varepsilon}^{(i)}(y_1,...,y_N) = \sum_{j=1}^N m_j \int_{\mathbb{R}^d} \nabla \zeta_{\varepsilon}(y_i-z) \zeta_{\varepsilon}(z-y_j) \frac{1}{\bar{\rho}(z)} \, dz - \nabla V_k(y_i).$$

Numerical method

- Discretize initial data into particles: $\rho_0 \approx \frac{1}{N} \sum_{i=1}^N \delta_{\chi_i^0}$.
- Let the particles evolve via the ODE system:

$$\frac{d}{dt}X_{j}(t) = -V_{\varepsilon}^{(j)}(X_{1}(t),...,X_{N}(t)), \quad X_{j}(0) = X_{j}^{0}.$$

Let

$$\rho_{\varepsilon,k}^{N}(x,t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_{i}(t)}.$$

• Consider "blobs" over each particle:

$$ilde{
ho}_{arepsilon,k}^{m{N}}(x,t) = rac{1}{N}\sum_{i=1}^{N}\zeta_{arepsilon}(x-X_i(t)) = (\zeta_{arepsilon}*
ho_{arepsilon,k}^{m{N}})(x,t).$$

• This $\tilde{\rho}_{\varepsilon,k}^{N}$ is our approximate solution.

Application to sampling

$$\partial_t \rho - \operatorname{div}\left(\rho \nabla\left(\frac{\rho}{\bar{
ho}}\right)\right) = 0 \text{ in } \Omega \times (0,\infty), \quad \partial_{\nu}\left(\frac{\rho}{\bar{
ho}}\right) = 0 \text{ on } (\partial\Omega) \times (0,\infty).$$

• Fact:
$$W_2(
ho(t), \mathbb{1}_{\overline{\Omega}}ar{
ho}) o 0$$
 as $t o \infty$.

Given

- target probability measure ρ̄,
 reference ρ₀ = ¹/_N Σ^N_{i=1} δ_{X⁰_i}.

Goal: find $\rho_N = \frac{1}{N} \sum_{i=1}^N \delta_{X_i}$ approximating $\bar{\rho}$.

• We prove, under the same assumptions as the main theorems:

Corollary

There exist
$$k = k(t) \rightarrow +\infty$$
, $\varepsilon = \varepsilon(k) \rightarrow 0$, and $N = N(\varepsilon) \rightarrow +\infty$ so that

$$\lim_{t\to+\infty}W_1\left(\rho_{\varepsilon,k}^N(\cdot,t),\mathbb{1}_{\overline{\Omega}}\overline{\rho}\right)=0.$$

• So, Corollary gives a way to approximate $\bar{\rho}$ by an empirical measure.

Numerical method

Videos!

Convergence of numerical method

Assumptions:

- $\Omega \subset \mathbb{R}^d$ is convex;
- **2** $\bar{\rho} \in C^1(\Omega)$ is bounded from above and away from zero on Ω ;
- **(a)** $\bar{\rho}$ log-concave on Ω , i.e $\bar{\rho}(x) = e^{\Phi(x)}$ for some Φ that's concave on Ω .
- mild assumptions on initial data ρ_0 .

Theorem (Craig, Elamvazhuthi, Haberland, T (2023))

Let ρ solve the PDE (D) with initial data ρ_0 . Then as $k \to \infty$, there exist subsequences $\varepsilon(k) \to 0$ and $N(k) \to \infty$, such that,

$$ho_{arepsilon,k}^{\sf N}(t)
ightarrow
ho(t)$$
 and $ilde{
ho}_{arepsilon,k}^{\sf N}(t)
ightarrow
ho(t)$,

in the 1-Wassertein distance*, uniformly in $t \in [0, T]$.

(*) hence also in the sense of "integrating against test functions"

Results on GF

Recall

$$\mathcal{F} = \mathcal{E} + \mathcal{V}_{\Omega}, \quad \mathcal{F}_{\varepsilon,k} = \mathcal{E}_{\varepsilon} + \mathcal{V}_{k}.$$

Under the same assumptions:

Theorem (Craig, Elamvazhuthi, Haberland, T (2023))

Let $\rho_{\varepsilon,k}$ be the Wasserstein gradient flow of $\mathcal{F}_{\varepsilon,k}$ with initial data ρ_0 . Then as $k \to \infty$, there exists a subsequence $\varepsilon(k) \to 0$ such that such that,

 $\rho_{\varepsilon,k}(t) \to \rho(t),$

in the 1-Wassertein distance, uniformly in $t \in [0, T]$, where ρ is the gradient flow of \mathcal{F} with initial data ρ_0 .

• The previously stated result follows from this.

Elements of the proof

- **4** AGS: Wasserstein GFs for $\mathcal{F} = \mathcal{E} + \mathcal{V}_{\Omega}$ are well-defined.
- **2** We show: GF for $\mathcal{F}_{\varepsilon,k} = \mathcal{E}_{\varepsilon} + \mathcal{V}_k$ are well-defined.
 - $\mathcal{E}_{\varepsilon}$ is λ_{ε} -convex along generalized geodesics in Wasserstein space (where $\lambda_{\varepsilon} < 0$ and $\lambda_{\varepsilon} \to -\infty$ as $\varepsilon \to 0$).
 - does not require log-concavity assumption.
- **③** Γ -convergence of $\mathcal{F}_{\varepsilon,k}$ to \mathcal{F} .
- **(**) Obtain estimate on an " H^1 -like norm" for GFs of $\mathcal{F}_{\varepsilon,k}$ that is uniform in ε .
 - key ingredient: energy estimate for the ε -PDE.
- **Ο** Γ-convergence of metric slopes of $\mathcal{F}_{\varepsilon,k}$ to those of \mathcal{F} .
- Solution Conclude via a general result (variant of Serfaty, 2011) on convergence of GF:

$$\underbrace{\mathcal{F}_{\varepsilon,k}(\rho_{\varepsilon,k}(0)) - \mathcal{F}_{\varepsilon,k}(\rho_{\varepsilon,k}(t))}_{\text{use step 3}} \geq \frac{1}{2} \underbrace{\int_{0}^{t} |\rho_{\varepsilon,k}'|^{2}(r)dr}_{\text{use compactness}} + \underbrace{\frac{1}{2} \int_{0}^{t} |\partial \mathcal{F}_{\varepsilon,k}|^{2}(\rho_{\varepsilon,k}(r))dr}_{\text{use step 5}}.$$

More on the proof: H^1 -like bound

Lemma

Suppose ρ is a solution to

$$\partial_t \rho - \mathsf{div}\left(\rho \nabla \left(\zeta_\varepsilon \ast \left(\frac{\zeta_\varepsilon \ast \rho}{\bar{\rho}}\right)\right)\right) = 0.$$

Then we have,

$$\int_0^T \int |\nabla \rho * \zeta_\varepsilon|^2 \, dx \, dt \le C.$$

Follows from energy estimate:

$$\frac{d}{dt}\int\rho\log(\rho)\,d\mathsf{x}+\int|\nabla\rho\ast\zeta_{\varepsilon}|^{2}=\langle\nabla\rho\ast\zeta_{\varepsilon},(\rho\ast\zeta_{\varepsilon})\nabla\left(\frac{1}{\bar{\rho}}\right)\rangle.$$

Energy estimate with $\bar{\rho} \equiv 1$:

$$\partial_t \rho - \operatorname{div}(\rho(\nabla \rho * \zeta_{\varepsilon} * \zeta_{\varepsilon})) = 0.$$
Note: $\frac{d}{dt} \int \rho \log(\rho) \, dx = \frac{d}{dt} \left(\int \rho \log(\rho) \, dx - \int \rho \, dx \right)$, so that,
 $\frac{d}{dt} \int \rho \log(\rho) \, dx = \int \rho_t \log(\rho) + \rho \frac{\rho_t}{\rho} - \rho_t \, dx$
 $= \int \operatorname{div}(\rho(\nabla \rho * \zeta_{\varepsilon} * \zeta_{\varepsilon})) \log(\rho) \, dx$
 $= -\int \rho(\nabla \rho * \zeta_{\varepsilon} * \zeta_{\varepsilon}) \nabla \log(\rho) \, dx$
 $= -\int \rho(\nabla \rho * \zeta_{\varepsilon} * \zeta_{\varepsilon}) \frac{\nabla \rho}{\rho} \, dx$
 $= -\int (\nabla \rho * \zeta_{\varepsilon} * \zeta_{\varepsilon}) \nabla \rho \, dx = -\int (\nabla \rho * \zeta_{\varepsilon})^2 \, dx.$

Recall: if ζ is even, then

$$\int (f * \zeta)(x)g(x)\,dx = \int f(x)(\zeta * g)(x)\,dx.$$

Thank you!