

Gradient Flows: An Overview

Gradient Flows Seminar

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Gradient Flows: The Smooth Setting

An Introduction to Gradient Flows

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Why do we care about gradient flows?

- 1 They describe important physical processes (e.g. the heat equation, the porous medium equation, etc.)
- 2 They play an important role in optimization algorithms.
- 3 They have a rich mathematical structure for proving well-posedness and understanding longtime behavior of many PDEs.

The Smooth Setting: Energy and Geometry

Consider

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- 2 a metric tensor g on $\mathcal{M}$, which makes $\mathcal{M}$ a Riemannian manifold,
- 3 and a differentiable function(al) $E : \mathcal{M} \rightarrow \mathbb{R}$.

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We start by defining two important objects:

- 1 $\text{diff}[E, x] : \text{Tan}_x \mathcal{M} \rightarrow \mathbb{R}$ is the differential of E , which takes in a direction at x and outputs the rate of change of E in that direction.
- 2 $\text{grad}[E, x] \in \text{Tan}_x \mathcal{M}$ is the unique element of $\text{Tan}_x \mathcal{M}$ such that for all $v \in \text{Tan}_x \mathcal{M}$,

$$g(\text{grad}[E, x], v) = \text{diff}[E, x](v).$$

Note that this variable depends on g !

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The **gradient flow** of E on $(\mathcal{M}, g)$ is the function $x : [0, \infty) \rightarrow \mathcal{M}$ that satisfies

$$\partial_t x(t) = -\text{grad}[E, x(t)].$$

Existence and uniqueness of such a flow is not guaranteed.

Energy Dissipation

How do we know that the gradient flow $\partial_t x(t) = -\text{grad}[E, x(t)]$ decreases the energy?

Assume that x is a smooth solution to the gradient flow. Then

$$\begin{aligned} \frac{d}{dt} E(x(t)) &= \text{diff}[E, x(t)](\dot{x}(t)) \\ &= g(\text{grad}[E, x(t)], \dot{x}(t)) \\ &= -g(\dot{x}(t), \dot{x}(t)) \\ &\leq 0. \end{aligned}$$

In other words, the energy decreases along the flow. However, energy decrease alone does not characterize a gradient flow.

Example: The Heat Equation

Formally, we consider

$$\mathcal{M} = \left\{ \rho : \mathbb{R}^d \rightarrow [0, \infty) : \int \rho = 1 \right\} \Rightarrow \text{Tan}_\rho \mathcal{M} = \left\{ v : \mathbb{R}^d \rightarrow \mathbb{R} : \int v = 0 \right\}.$$

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We define

$$E(\rho) = \frac{1}{2} \int \rho^2.$$

Let us calculate the differential (which does not depend on the metric tensor g):

$$\begin{aligned} \text{diff}[E, \rho](v) &= \lim_{t \rightarrow 0} \frac{E(\rho + tv) - E(\rho)}{t} \\ &= \lim_{t \rightarrow 0} \frac{1}{2t} \int (\rho + tv)^2 - \rho^2 \\ &= \lim_{t \rightarrow 0} \frac{1}{2t} \int 2\rho tv + t^2 v^2 \\ &= \int v \rho. \end{aligned}$$

The Heat Equation Continued: Adding a Metric Tensor

Fix $\rho \in \mathcal{M}$, and choose $v_1, v_2 \in \text{Tan}_\rho \mathcal{M}$. We may choose $u_1, u_2 \in \mathbb{R}^d \rightarrow \mathbb{R}$ such that $-\Delta u_i = v_i$. Define

$$g(v_1, v_2) = \int \nabla u_1 \cdot \nabla u_2 = \int v_2 u_1.$$

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We seek $G := \text{grad}[E, \rho]$, the unique element of $\text{Tan}_\rho \mathcal{M}$ such that for all $v \in \text{Tan}_\rho \mathcal{M}$,

$$g(G, v) = \text{diff}[E, \rho](v).$$

If we define p_G such that $-\Delta p_G = G$, the above equality reduces to $\int v p_G = \int v \rho$ for all $v : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $\int v = 0$.

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This implies that $p_G = \rho + C$, i.e. $\text{grad}[E, \rho] = G = -\Delta p_G = -\Delta \rho$. Thus, the gradient flow is

$$\partial_t \rho = -\text{grad}[E, \rho] = \Delta \rho,$$

i.e. the heat equation!

Extending to the Metric Setting

The Minimizing Movement Scheme on Euclidean Space

Suppose we want to solve a gradient flow equation. A standard variational way to calculate a solution is via a **minimizing movement scheme** (MMS).

First, we consider the case $\mathcal{M} = \mathbb{R}^d$ equipped with the classical inner product. In this case, the gradient flow $x : [0, T] \rightarrow \mathbb{R}^d$ of an energy functional $E : \mathbb{R}^d \rightarrow \mathbb{R}$ is

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Given x^k and $\tau > 0$, assuming a minimizer exists, choose

$$x^{k+1} \in \operatorname{argmin}_{y \in \mathbb{R}^d} \left\{ E(y) + \frac{|y - x^k|^2}{2\tau} \right\}.$$

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Motivation: If E is differentiable, a minimizer satisfies

$$0 = \nabla E(x^{k+1}) + \frac{x^{k+1} - x^k}{\tau} \Rightarrow x^{k+1} = x^k - \tau \nabla E(x^{k+1}),$$

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Under suitable assumptions, the interpolated discrete solutions converge, possibly along a subsequence, to a gradient-flow solution as $\tau \rightarrow 0$.

Minimizing Movements Beyond Euclidean Space

Let (M, g) be a Riemannian manifold, and let d_g be its induced distance.

Given x^k and $\tau > 0$, assuming a minimizer exists, choose

$$x^{k+1} \in \operatorname{argmin}_{y \in M} \left\{ E(y) + \frac{d_g(y, x^k)^2}{2\tau} \right\}.$$

Only the energy and the distance enter this construction. The same formula therefore makes sense on a general metric space (X, d) .

Again, we interpolate the iterates and study the limit as $\tau \rightarrow 0$.

The Energy Dissipation Equality in Euclidean Space

Young's inequality: For $u, v \in \mathbb{R}^d$, $u \cdot v \leq \frac{1}{2} (|u|^2 + |v|^2)$. Equality holds iff $u = v$.

Suppose the curve $x : [0, T] \rightarrow \mathbb{R}^d$ and energy $E : \mathbb{R}^d \rightarrow \mathbb{R}$ are both sufficiently smooth. By Young's inequality,

$$E(x(s)) - E(x(t)) = \int_s^t -\nabla E(x(r)) \cdot x'(r) dr \leq \frac{1}{2} \int_s^t (|\nabla E(x(r))|^2 + |x'(r)|^2) dr.$$

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The **Energy Dissipation Equality** in Euclidean space: For $s < t$,

$$E(x(s)) - E(x(t)) = \frac{1}{2} \int_s^t (|\nabla E(x(r))|^2 + |x'(r)|^2) dr.$$

How do we extend this to the general metric setting?

The Slope of the Energy and Metric Derivative

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A curve $x : [0, T] \rightarrow X$ is **absolutely continuous** if there exists a nonnegative $m \in L^1(0, T)$ such that for $0 \leq s < t \leq T$,

$$d(x(s), x(t)) \leq \int_s^t m(r) \, dr.$$

If m can be chosen in $L^2(0, T)$, write $x \in AC^2([0, T]; X)$. For absolutely continuous curves, the metric derivative exists almost everywhere.

The EDE in a General Metric Space

In Euclidean space, the EDE is

$$E(x(s)) - E(x(t)) = \frac{1}{2} \int_s^t \left(|\nabla E(x(r))|^2 + |x'(r)|^2 \right) dr.$$

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In the general metric space, we replace $|\nabla E(x)|$ with the slope of the energy $|\nabla^- E|(x)$ and we replace $|x'(r)|$ with the metric derivative $|x'|_|(r)$:

$$E(x(s)) - E(x(t)) = \frac{1}{2} \int_s^t \left(|\nabla^- E(x(r))|^2 + |x'|_|(r)^2 \right) dr.$$

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An AC^2 -curve $x : [0, T] \rightarrow X$ is an **EDE solution** if, for every $0 \leq s < t \leq T$, the equality above is satisfied.

The Evolution Variational Inequality in Euclidean Space

Suppose the curve $x : [0, T] \rightarrow \mathbb{R}^d$ and energy $E : \mathbb{R}^d \rightarrow \mathbb{R}$ are both sufficiently smooth.

First, notice that

$$\frac{d}{dt} \frac{1}{2} |x(t) - y|^2 = -x'(t) \cdot (y - x(t)). \quad (1)$$

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As a result, if E is λ -convex,

$$\begin{aligned} x'(t) &= -\nabla E(x(t)) \\ &\iff -x'(t) \in \partial E(x(t)) \\ &\iff \forall y \in \mathbb{R}^d, E(y) \geq E(x(t)) + \frac{\lambda}{2} |x(t) - y|^2 - x'(t) \cdot (y - x(t)) \\ &\iff \forall y \in \mathbb{R}^d, E(y) \geq E(x(t)) + \frac{\lambda}{2} |x(t) - y|^2 + \frac{d}{dt} \frac{1}{2} |x(t) - y|^2 \\ &\iff \forall y \in \mathbb{R}^d, \frac{d}{dt} \frac{1}{2} |x(t) - y|^2 \leq E(y) - E(x(t)) - \frac{\lambda}{2} |x(t) - y|^2. \end{aligned}$$

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Thus, in the Euclidean setting, $x(t)$ is a gradient flow of (a λ -convex functional) E iff the EVI condition is satisfied. Notice that the EVI expression is still well-defined in the general metric setting.

The EVI in a General Metric Space

Let (X, d) be a metric space, let $E : X \rightarrow \mathbb{R}$, and fix $\lambda \in \mathbb{R}$. An absolutely continuous curve $x : [0, T] \rightarrow X$ satisfies the **Evolution Variational Inequality** EVI_λ if for every fixed $y \in X$, $y \neq x$, and for almost every t ,

$$\frac{1}{2} \frac{d}{dt} d(x(t), y)^2 \leq E(y) - E(x(t)) - \frac{\lambda}{2} d(x(t), y)^2.$$

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Suppose x and $\tilde{x}$ satisfy EVI_λ for the same energy and metric. Then

$$d(x(t), \tilde{x}(t))^2 \leq e^{-2\lambda t} d(x(0), \tilde{x}(0))^2.$$

This implies uniqueness for a prescribed initial condition.

Furthermore, if $\lambda > 0$, then we obtain exponential contraction of the two curves.

Geodesic Convexity

Let (X, d) be a metric space and let $E : X \rightarrow \mathbb{R}$.

A curve $x : [0, 1] \rightarrow X$ is a **constant-speed geodesic** if for all $0 \leq s, t \leq 1$,

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We say that E is **λ -geodesically convex** if for every $x_0, x_1 \in X$, there exists a constant-speed geodesic x connecting x_0 to x_1 such that for all $0 \leq s \leq 1$,

$$E(x(s)) \leq (1 - s)E(x_0) + sE(x_1) - \frac{\lambda}{2}s(1 - s)d(x_0, x_1)^2.$$

Geodesic Convexity, EDE, and EVI

If E is λ -geodesically convex,

- 1 If $\lambda \geq 0$, every finite-energy local minimizer is a global minimizer.
- 2 If $\lambda > 0$ and E has a minimizer x_* , then x_* is unique.

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Under suitable lower-semicontinuity and compactness assumptions:

- 1 Minimizing-movement limits for a λ -geodesically convex energy satisfy EDE.
- 2 Every EVI_λ solution satisfies EDE, but the converse is false in general.
- 3 EVI gives uniqueness and stability; EDE alone need not give uniqueness.

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