

On the global convergence of gradient descent using optimal transport

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Introduction to Real Analysis II, Prof. G. Savaré

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Overview

Introduction

Problem re-formulation

Apply gradient flow theory

Particle gradient flow

Generalize to infinite-dimensional gradient flow

Global convergence guarantees

References

Introduction

Classical task in machine learning:

$$\min_{\mu \in \mathcal{P}(\Theta)} j(\mu) \quad j(\mu) = \ell \left(\int \phi \, d\mu \right) + g(\mu) \quad (1)$$

$\ell : \mathcal{F} \rightarrow \mathbb{R}_+$ smooth, convex *loss function*

data lives in a large parametrized set with parameters $p \in \Theta \subset \mathbb{R}^d$

$g : \mathcal{P}(\Theta) \rightarrow \mathbb{R}$ optional convex *regularizer*

we look for a linear combination ϕ mapping features to labels

$$\phi(p) : x \mapsto \sigma(\sum_i p_i x_i + p_d), p \in \Theta$$

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★ Minimize over the space of measures $\mathcal{P}(\Theta)$ ★

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Convex problem, but intractable

⇒ discretize the measure into m particles parametrized by *weights* and *positions*

$$\mu_m := \frac{1}{m} \sum_{i=1}^m w_i \delta_{p_i}$$

$$\min_{\substack{w \in \mathbb{R} \\ p \in \Theta^m}} j_m(w, p) \quad j_m(w, p) := j(\mu_m) \quad (2)$$

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Non-convex problem

* Idea: use tools from optimal transport to exploit convexity of (1) to study global convergence in (2) *

Conceptual key points

1. Problem reformulation (lifting) $j \rightarrow f$
2. To be able to study gradient flow of $f_m, (\mu_{m,t})_t$
3. Look at it as a particular case of infinite-dimensional case

as $m \rightarrow \infty, (\mu_{m,t})_t \rightarrow (\mu_t)_t$

4. Exploit convex structure of inf-dim case

$$\lim_{m,t \rightarrow \infty} f(\mu_{m,t}) = \min_{\mu_t \in \mathcal{P}(\Omega)} f(\mu_t)$$

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Lifting

$$\min_{\nu \in \mathcal{P}(\Theta)} j(\nu) = \ell \left(\int \phi \, d\nu \right) + g(\nu) \quad (1)$$

$$\downarrow h_1^{-1}$$

$$\min_{\mu \in \mathcal{P}(\Omega)} f(\mu) = \ell \left(\int \varphi \, d\mu \right) + \int v \, d\mu \quad (3)$$

Recovering the lifting:

- ▶ $\Omega = \Theta \times \mathbb{R}$
- ▶ $\varphi(p, w) = w\phi(p)$
- ▶ projection map: $h_1 : \Theta \times \mathbb{R} \rightarrow \Theta$, $h_1(\mu)(p) = \int_{\mathbb{R}} w\mu(dw, p)$
- ▶ $g(\nu) = \inf_{\mu \in h_1^{-1}(\nu)} \int v \, d\mu$
- ▶ then, $\inf_{\nu} j = \inf_{\mu} f$

New problem

$$\min_{\mu \in \mathcal{P}(\Omega)} f(\mu) = \ell \left(\int \varphi \, d\mu \right) + \int v \, d\mu$$

Discretized problem:

$$\min_{u \in \Omega} f_m(u) := f \left(\underbrace{\frac{1}{m} \sum_{i=1}^m \delta_{u_i}}_{\mu_m} \right) = \ell \left(\frac{1}{m} \sum_{i=1}^m \varphi(u_i) \right) + \frac{1}{m} \sum_{i=1}^m v(u_i)$$

- ★ Weights w are another coordinate of a particle position $u \in \Omega$
- ⇒ study gradient flow of f_m ★

New problem

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Assumptions (high-level):

- ▶ ℓ is smooth, with Lipschitz and bounded differential $d\ell$
- ▶ ϕ is differentiable and v is semiconvex
- ▶ there is a family of nested closed convex sets $(Q_r)_r$ on which the (sub)derivatives of ϕ, v are Lipschitz and grow sublinearly

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Prerequisites

Definition (Subgradient and subdifferential)

Given a function $f : \mathbb{R}^d \rightarrow \mathbb{R}$, the *subgradient of f at x_0* , $x_0 \in \mathbb{R}^d$, is $p \in \mathbb{R}^d$:

$$f(x) \geq f(x_0) + p \cdot (x - x_0) + o(x - x_0) \quad \forall x \in \mathbb{R}^d$$

The set of all such p s is called the *subdifferential of f at x_0* and we write $\partial f(x_0)$. The subdifferential is a closed and convex set.

Definition (Gradient flow)

A function $x : \mathbb{R}_+ \rightarrow \text{Dom}(f)$ is a *gradient flow of f* if x is absolutely continuous over \mathbb{R}_+ and

$$x'(t) \in -\partial f(x(t)) \quad \text{for a.e. } t \in \mathbb{R}_+$$

Particle gradient flow I

Definition (Particle gradient flow)

A gradient flow for f_m is an absolutely continuous function $u : \mathbb{R}_+ \rightarrow \Omega^m$ such that

$$u'(t) \in -m \partial f_m(u(t))$$

for almost every $t \in \mathbb{R}_+$.

Properties:

- (i) (existence and uniqueness) for any $u(0) \in \Omega^m$ starting point, there exists a unique gradient flow for f_m
- (ii) (derivative of f_m) for a.e. $t \in \mathbb{R}_+$, it holds

$$\frac{d}{ds} f_m(u(s)) \Big|_{s=t} = -|u'(t)|^2$$

Particle gradient flow II

(iii) (form of the velocity) the velocity of the i -th particle $u_i(t)$ is a vector field $v_t : \Omega \rightarrow \mathbb{R}^d$ given by $u'_i(t) = v_t(u_i(t))$ where [2]

$$v_t(u_i) = \tilde{v}_t(u_i) - \text{proj}_{\partial v(u_i)}(\tilde{v}_t(u_i))$$

$$\text{with } \tilde{v}_t(u_i) = - \left[\left(\ell' \left(\int \varphi \, d\mu_{m,t} \right), \partial_j \varphi(u_i) \right) \right]_{j=1}^d$$

from [2], gradient flow selects subgradients of minimal norm
Observations:

- ▶ velocity is the evaluation at each u_i of the same vector field v_t
 - ▶ given an initialization $u(0) \in \Omega^m$, this defines an atomic measure $\mu_{m,0}$
- makes sense to generalize to arbitrary measures μ_t

Generalize to Wasserstein gradient flow I

Since

1. Evolution of $(\mu_t)_t$ under $(v_t)_t$ satisfies:

$$\partial_t \mu_t = -\operatorname{div}(v_t \mu_t)$$

2. Link between v_t and f :

$$v_t \in -\partial f'(\mu_{m,t})$$

$$\text{where } f'(\mu)(u) := \left(\ell \left(\int \varphi \, d\mu \right), \varphi(u) \right) + v(u)$$

⇒ we expect $(\mu_t)_t$ is a gradient flow on the space $\mathcal{P}_2(\Omega)$:
Wasserstein gradient flow

Generalize to Wasserstein gradient flow II

Definition (Wasserstein gradient flow)

A Wasserstein gradient flow for the functional f on a time interval $[0, T[$ is an absolutely continuous path $(\mu_t)_{t \in [0, T[}$ in $\mathcal{P}_2(\Omega)$ that satisfies, distributionally on $[0, T[\times \Omega^d$,

$$\partial_t \mu_t = -\operatorname{div}(v_t \mu_t) \quad \text{where } v_t \in -\partial f'(\mu_t)$$

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W_2 gradient flow generalizes particle

Whenever $(u_t)_t$ is a gradient flow for f_m , $t \mapsto \mu_{m,t} := \sum_{i=1}^m \delta_{u_i(t)}$ is a Wasserstein gradient flow for f !

Many-particle limit

Theorem (Many particle limit)

Consider $(t \mapsto u_m(t))_{m \in \mathbb{N}}$ a sequence of classical gradient flows for f_m initialized in a closed convex set. If $\mu_{m,0}$ converges to some $\mu_0 \in \mathcal{P}_2(\Omega)$ for the Wasserstein distance W_2 , then $(\mu_{m,t})_t$ converges, as $m \rightarrow \infty$, to the unique Wasserstein gradient flow of f starting from μ_0 .

In a nutshell:

- ▶ if $u(0) = (u_1(0), \dots, u_m(0))$ are distributed according to μ_0 , then $\mu_{m,0}$ converges to μ_0 by the law of large numbers
- ▶ $\lim_{m \rightarrow \infty} (\mu_{m,t})_t = (\mu_t)_t$

Global convergence result

Structural assumptions:

- ▶ φ, v are **2-homogeneous** (ϕ 1-homogeneous)
- ▶ the support of the initialization of the Wasserstein gradient flow satisfies a “**separation**” **property**: $B(0, r_b) \subset \mathbb{S}^{d-1}$ that separates $r_a \mathbb{S}^{d-1}$ and $r_b \mathbb{S}^{d-1}$ for $r_a < r_b$

Theorem (Global convergence of particle gradient descent)

Let $(\mu_t)_{t \geq 0}$ be a Wasserstein gradient flow of f such that the support of μ_0 is $S_0 \subset [-r_0, r_0] \times \Theta$ satisfies a separation property. If $(\mu_t)_t$ converges to μ_∞ in W_2 , then μ_∞ is a global minimizer of f over $\mathcal{P}(\Omega)$. In particular, if $(u_m(t))_{m \in \mathbb{N}, t \geq 0}$ is a sequence of classical gradient flows initialized in $[-r_0, r_0] \times \Theta$ such that $\mu_{m,0}$ converges to μ_0 in W_2 then

$$\lim_{t,m \rightarrow \infty} f(\mu_{m,t}) = \min_{\mu \in \mathcal{P}(\Omega)} f(\mu).$$

Application to ReLu neural networks

Setting:

- ▶ features live in \mathbb{R}^{d-2} , labels in \mathbb{R}
- ▶ ℓ is either the square or logistic loss
- ▶ 2-homogeneous case
- ▶ domain Θ is the disjoint union of 2 copies of \mathbb{R}^d
- ▶ $\varphi(p) : x \mapsto \sigma(\sum_{i=1}^{d-1} s(p_i)x_i + s(p_d))$, $s(p_i) = p_i|p_i|$
- ▶ regularizer: $v(p) = |p|^2$ (as if $w = |p|$)

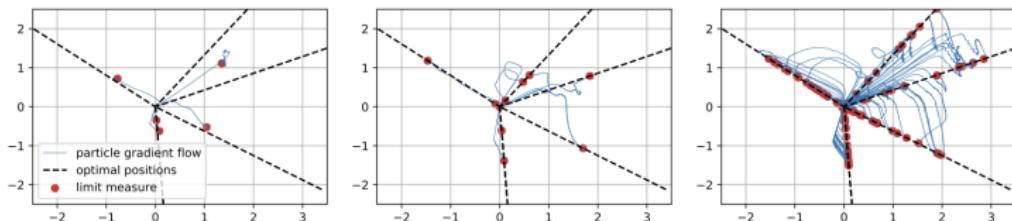


Figure: Training neural network with ReLU activation. Overfitting threshold $m = 4$. Failure for $m = 5$, success $m = 10, 100$.

Final remarks

- ▶ importance of initialization, as confirmed by extensive empirical literature
- ▶ particle gradient flow corresponds to continuous-time gradient descent: what can we say about discrete-step case? (double descent)

Thank you!



References I

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Recovering the lifting of (3)

1. (equivalence of \mathcal{M} and \mathcal{P} under homogeneity)
2. surjectivity of h_1
3. define φ, g as above and prove equality of f, j