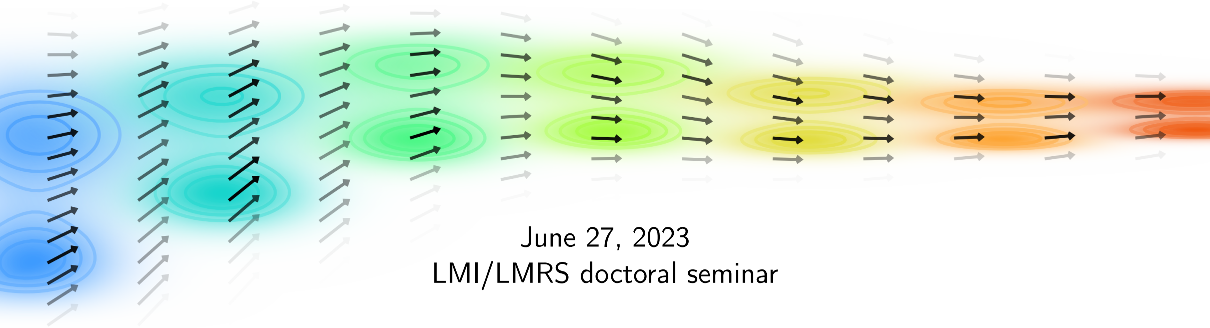
The D in PDE

Strategies for first-order differentiation in the space of measures

Averil Prost



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$$\partial_t u(t,\mu) + \langle \partial_\mu u(t,\mu), b\rangle = 0, \qquad u(0,\mu) = u_0(\mu)$$

admits as solution $u(t,\mu) = u_0\left((id - tb)\#\mu\right)$.

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This talk will review the definitions of the literature, going from smoothest to most general.

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Some definitions

Let $\mathcal{D} := \mathcal{C}_c^1\left(\mathbb{R}^d, \mathbb{R}\right)$. For each initial measure μ, denote $(\mu_s^{\mu,p})_{s\geqslant 0}$ the unique solution of the continuity equation

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Def 1 – Distributional derivative A map $u : \mathscr{P}(\mathbb{R}^d) \to \mathbb{R}$ admit a distributional derivative if there exist a distribution $\text{grad}_\mu u \in \mathcal{D}'$ such that for all $p \in \mathcal{D}$,

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This definition is used in [FK09, FN12] to adress Hamilton-Jacobi equations.

Example: the linear map

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Remark 1 – Meaning of the divergence Here $\text{div } (\mu\cdot)$ is a *notation* for the adjoint operator of the gradient, i.e. $\langle \text{div}\, (\mu F), p\rangle := \langle F, \nabla p\rangle_\mu = \int_{x\in\mathbb{R}^d} \langle F(x), \nabla p(x)\rangle \, d\mu(x)$. In particular, if μ is the Lebesgue measure, it contains the boundary terms.

The Otto calculus

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Hence $\operatorname{grad}_\mu u = -\operatorname{div}\left(\rho\nabla[U'\circ\rho]\right)$. For instance, $U(r) = r\ln(r)$ gives $\operatorname{grad}_\mu u = -\Delta\rho(x)$.

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Fundamental theorem of simulation (name from [BL94], [CD18a, Lemma 5.29])
Let $(\Omega, \mathcal{A}, \mathbb{P})$ be an atomless probability space, and $\mu \in \mathscr{P}_2\left(\mathbb{R}^d\right)$. Then there exist $X \in L^2\left(\Omega, \mathcal{A}, \mathbb{P}; \mathbb{R}^d\right)$ such that

the law of X is μ, i.e. $\mu = X\#\mathbb{P}$, i.e. $\mu(A) = \mathbb{P}(X^{-1}(A)) \quad \forall A \in \mathcal{A}$.

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Def 2 – Lift Let $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$. Its *lift* is a map $U : L^2\left(\Omega, \mathcal{A}, \mathbb{P}; \mathbb{R}^d\right) \to \mathbb{R}$ given by

$$U(X) = u(\mathcal{L}(\mathcal{X})) = u(X\#\mathbb{P}).$$

Gradient using the Hilbert structure

Def 3 – L-derivative Assume that U is F-differentiable in $L^2\left(\Omega, \mathcal{A}, \mathbb{P}; \mathbb{R}^d\right)$. Then for all $\mu \in \mathscr{P}_2(\mathbb{R}^d)$, there exist an element $\xi_\mu \in L^2_\mu\left(\mathbb{R}^d; \mathbb{R}^d\right)$ such that

$$\forall X \in L^2\left(\Omega, \mathcal{A}, \mathbb{P}; \mathbb{R}^d\right) \text{ s.t. } \mathcal{L}(X) = \mu, \qquad \nabla U(X)(\omega) = \xi_\mu(X(\omega)) \quad \forall \omega \in \Omega.$$

We then denote $\partial_\mu u(\mu) := \xi_\mu$. (Here, $\partial_\mu u(\mu)$ is a function in $L^2_\mu(\mathbb{R}^d; \mathbb{R}^d)$.)

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Idea launched by P.L. Lions in [Lio06], transcripted in [Car13]. Very popular notion, used (in particular) in [CCD15, PW17, PW18, BY19, CGK$^+$22, CGK$^+$22, MZ22] to make the link between SDEs and PDEs, with focus on the master equation. Higher order derivatives are also defined (see [Sal23] for arbitrary order).

Example

Consider again $u(\mu) := \int_{x\in\mathbb{R}^d} \ell(x) d\mu(x)$. Then its lift U is defined as

$$U(X) = \int_{\omega\in\Omega} \ell(X(\omega)) d\mathbb{P}(\omega).$$

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If $\ell \in \mathcal{C}^1$ and Lipschitz, then

$$\lim_{h\searrow 0} \frac{U(X+hY)-U(X)}{h} = \int_{\omega\in\Omega} \langle \nabla\ell(X(\omega)), Y(\omega)\rangle \, d\mathbb{P}(\omega) = \langle \nabla\ell \circ X, Y\rangle_{L^2_{\mathbb{P}}}.$$

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Hence $DU(X) = \nabla\ell\circ X$, and $\partial_\mu u(\mu) = \nabla\ell : \mathbb{R}^d \to \mathbb{R}^d$ (here independant of μ).

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Remark 2 – Insatisfaction This "delocalization" procedure does not seem really natural.

The linear derivative

Def 4 – Linear derivative A map $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$ is said to admit a linear (functional) derivative if there exist a function $(\mu, x) \mapsto \frac{\delta u}{\delta \mu}(\mu, x)$ satisfying

- for all $\nu \in \mathscr{P}_2(\mathbb{R}^d)$, $\lim_{s \searrow 0} \frac{u(\mu+s(\nu-\mu))-u(\mu)}{s} = \int_{x\in\mathbb{R}^d} \frac{\delta u}{\delta \mu}(\mu, x) d\left[\nu - \mu\right](x)$,

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- the normalizing convention $\int_{x\in\mathbb{R}^d} \frac{\delta u}{\delta \mu}(\mu, x) d\mu(x) = 0$.

This formulation goes back to Fleming-Viot processes [FV79], and is used outside of the Wasserstein context (see [CLS18] for references). It corresponds to the Fréchet derivative in the Banach space $(\mathcal{M}, |\cdot|_{TV})$, restricted to $\mathscr{P}_2(\mathbb{R}^d)$. Used in viscosity [BIRS19] and for the master equation [CD18a, CDLL19].

Example and chain rule

Let $u(\mu) := \int_{x\in\mathbb{R}^d} \ell(x)d\mu(x)$. Then one simply has

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Chain rule 1 If $(x,\mu) \mapsto \frac{\delta u}{\delta \mu}(\mu, x)$ is Lipschitz in $\mathscr{P}_2(\mathbb{R}^d) \times \mathbb{R}^d$ and the curve $(\mu_t)_{t\in[0,T]} \subset \mathscr{P}_2(\mathbb{R}^d)$ is Lipschitz in time, then

$$u(\mu_T) - u(\mu_0) = \int_{t=0}^{T} \langle \frac{\delta u}{\delta \mu}(\mu_t, \cdot), \partial_t \mu_t \rangle dt. \qquad \text{(CR-}\delta/\delta\mu\text{)}$$

The (natural) derivative

Def 5 – Natural derivative Assume that $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$ admits a linear derivative that is jointly continuous, and such that for all fixed $\mu \in \mathscr{P}_2(\mathbb{R}^d)$, the map $x \mapsto \frac{\delta u}{\delta \mu}(\mu, x)$ is differentiable in $\mathbb{R}^d$. Then one defines the natural derivative of u as

$$D_\mu u : \mathscr{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}^d, \qquad D_\mu u(\mu, x) = \nabla_x \frac{\delta u}{\delta \mu}(\mu, x).$$

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The notations are taken from [CD18a, CD18b], and this definition is used in [CDLL19]. The terminology is not clear, and we called $D_\mu u$ "natural derivative" in waiting of a better name.

Example and chain rule

According to Frame 12, the map $u(\mu) := \int_{x\in\mathbb{R}^d} \ell(x)d\mu(x)$ has a linear derivative $\frac{\delta u}{\delta\mu}(\mu,x) = \ell(x) - \langle \ell, \mu\rangle$. Hence we directly have

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$$D_\mu u(\mu,x) = \nabla_x \frac{\delta u}{\delta \mu}(\mu,x) = \nabla \ell(x).$$

Chain rule 2 Assume that $D_\mu u(\mu)$ is jointly continuous, and let the measure curve $(\mu_t)_{t\in[0,T]}$ solve $\partial_t \mu_t = -\operatorname{div}(g(t,\cdot,\mu_t)\#\mu_t)$. Then, from (CR-$\delta/\delta\mu$), we obtain

$$\begin{aligned} u(\mu_T) - u(\mu_0) &= \int_{t=0}^{T} \left\langle \nabla_x \frac{\delta u}{\delta\mu}(\mu,x), g(t,\cdot,\mu_t) \right\rangle_{\mu_t} dt \\ &= \int_{t=0}^{T} \int_{x\in\mathbb{R}^d} \langle D_\mu u(\mu_t,x), g(t,x,\mu_t)\rangle \, d\mu_t(x) dt. \end{aligned}$$

Links

Link ([CD18a, Prop. 5.48] and [CDLL19, Appx A]) Let $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$, and assume that either

- u admits a jointly continuous Lions-differential $\partial_\mu u$ in the sense of Def 3 that has linear growth in x uniformly in μ,
- u admits a jointly continuous natural derivative $D_\mu u$ in the sense of Def 5 that has linear growth in x uniformly in μ.

Then the other point stands and

$$\partial_\mu u(\mu, x) = D_\mu u(\mu, x) \qquad \forall (\mu, x) \in \mathscr{P}_2(\mathbb{R}^d) \times \mathbb{R}^d.$$

Hence the two definitions are gathered under the vocabulary of "Lions differentiability".

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The regular case

Define a family of "tangent vectors" to μ as

$$T_\mu \mathscr{P}_2(\mathbb{R}^d) := \overline{\{\nabla\varphi \mid \varphi \in \mathcal{C}_c^1(\mathbb{R}^d;\mathbb{R})\}}^{L^2_\mu}.$$

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Def 6 – Regular semidifferentials Let $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$ and $\mu \in \mathscr{P}_2(\mathbb{R}^d)$. An element $\xi \in T_\mu \mathscr{P}_2(\mathbb{R}^d)$ is said to belong to the subdifferential of u at μ if for all $\nu \in \mathscr{P}_2(\mathbb{R}^d)$,

$$u(\nu) - u(\mu) \geqslant \sup_{\eta \in \Gamma_o(\mu,\nu)} \int_{(x,y)\in(\mathbb{R}^d)^2} \langle \xi(x), y - x\rangle \, d\eta(x,y) + o\left(d_{\mathcal{W}}(\mu,\nu)\right).$$

The set of such ξ is denoted $\partial_{.} u(\mu)$. The superdifferential writes $\partial^{\cdot} u(\mu) := -\partial_{.}(-u)(\mu)$.

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This definition inspired the $\delta-$semidifferentials of [CQ08, MQ18, JMQ20, JMQ22].

Example

Let $u(\mu) = \int_{x \in \mathbb{R}^d} \ell(x) d\mu(x)$, and assume that $\ell \in \mathcal{C}^1$ is $\lambda-$semiconvex, i.e.

$$\ell(y) - \ell(x) \geqslant \langle \nabla \ell(x), y - x \rangle - \frac{\lambda}{2} |y - x|^2 .$$

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Then, for any $(\mu, \nu) \in (\mathscr{P}_2(\mathbb{R}^d))^2$, integrating the above against $\eta \in \Gamma_o(\mu, \nu)$ yields

$$\underbrace{\int_{y\in\mathbb{R}^d} \ell(y) d\nu(y)}_{u(\nu)} - \underbrace{\int_{x\in\mathbb{R}^d} \ell(x) d\mu(x)}_{u(\mu)} \geqslant \int_{(x,y)\in(\mathbb{R}^d)^2} \langle \nabla \ell(x), y - x \rangle \, d\eta(x, y) - \frac{\lambda}{2} d^2_{\mathcal{W}}(\mu, \nu).$$

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Since η is arbitrary, we conclude that $x \mapsto \nabla \ell(x)$ belongs to the subdifferential of u at μ.

Link with the Lions differentiability

Def 7 – W-differential Let $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$ such that $\partial_{\cdot} u(\mu) \neq \emptyset$ and $\partial^{\cdot} u(\mu) \neq \emptyset$. Then $\partial_{\cdot} u(\mu) = \partial^{\cdot} u(\mu) = \{\xi\}$, and the Wasserstein gradient of u at μ is $\nabla_W u(\mu) := \xi$.

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The map u admits a W-gradient $\nabla_W u(\mu)$ at μ if and only if its lift $U(X) := u(\mathcal{L}(X))$ is differentiable at some X such that $\mathcal{L}(X) = \mu$. In this case, one has $\nabla_W u(\mu) = \partial_\mu u(\mu)$.

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The geometric approach of Wasserstein gradients originated in [AGS05], followed by [GNT08]. [AG08, GŚ14] make a direct use of this definition in viscosity solutions. The above link was shown in [GT19, Corollary 3.22] (see also [CD18a, Theorem 5.64]).

The general tangent cone

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$$\boldsymbol{T}_\mu \mathscr{P}_2(\mathbb{R}^d) := \overline{\left\{\xi \in \mathscr{P}(T\mathbb{R}^d)_\mu \;\middle|\; \exists \varepsilon > 0, t \mapsto \exp_\mu(t \cdot \xi) \text{ is a geodesic on } t \in [0,\varepsilon]\right\}}^{W_\mu},$$

where $W_\mu(\xi,\eta) := \int_{x\in\mathbb{R}^d} d_{\mathcal{W}}(\xi_x,\eta_x) d\mu(x)$ is a generalization of the L^2_μ distance on plans.

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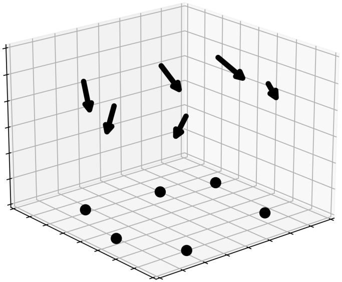

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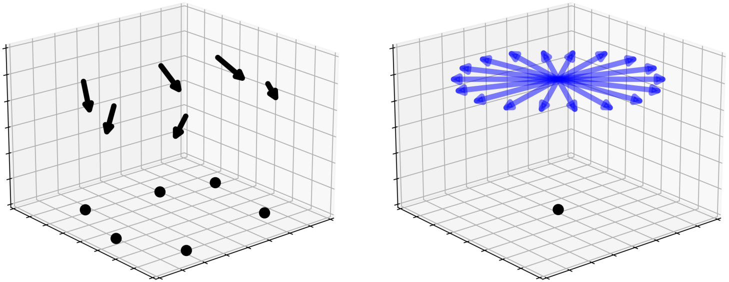

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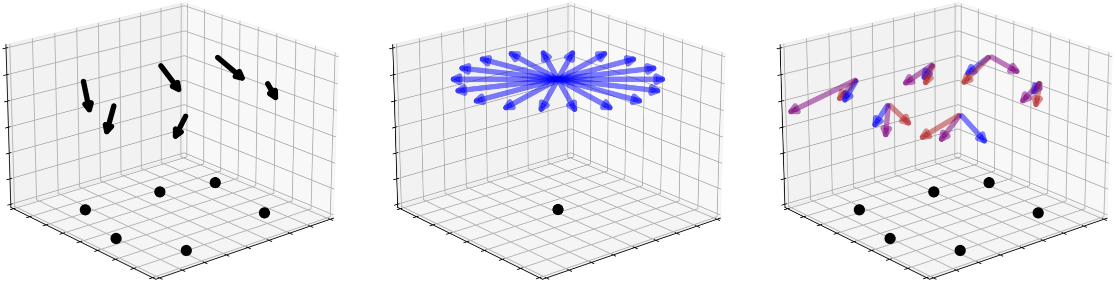

Generalized semidifferentials

For any $\xi \in \boldsymbol{T}_\mu \mathscr{P}_2(\mathbb{R}^d)$ and $\nu \in \mathscr{P}_2(\mathbb{R}^d)$, denote $\Gamma_o(\xi, \nu)$ the set of plans

$$\eta \in \mathscr{P}\left(\left\{(x, v_1, v_2) \;\middle|\; x \in \mathbb{R}^d, v_i \in T_x\mathbb{R}^d\right\}\right) \quad \text{s.t.} \quad \begin{cases} \pi_{x,v_1}\#\eta = \xi, \\ (\pi_x, \pi_x + \pi_{v_2})\#\eta \in \Gamma_o(\mu, \nu). \end{cases}$$

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Def 8 Let $u : \mathscr{P}_2(\mathbb{R}^d) \to \mathbb{R}$ and $\mu \in \mathscr{P}_2(\mathbb{R}^d)$. A tangent vector $\xi \in \boldsymbol{T}_\mu \mathscr{P}_2(\mathbb{R}^d)$ belongs to the generalized subdifferential of u at μ, denoted $\boldsymbol{\partial}_{.}u(\mu)$, if for all $\nu \in \mathscr{P}_2(\mathbb{R}^d)$,

$$u(\nu) - u(\mu) \geqslant \sup_{\eta \in \Gamma_o(\xi,\nu)} \int_{x \in \mathbb{R}^d, (v_1,v_2) \in (T_x\mathbb{R}^d)^2} \langle v_1, v_2 \rangle \, d\eta(x,v_1,v_2) + o\left(d_{\mathcal{W}}(\mu,\nu)\right),$$

The generalized superdifferential is defined as $\boldsymbol{\partial}^{\cdot}u(\mu) := -\boldsymbol{\partial}_{.}(-u)(\mu)$.

Example

Let $u(\mu) := \int_{x\in\mathbb{R}^d} \ell(x)d\mu(x)$, and assume that ℓ is $\lambda-$semiconvex (but not $\mathcal{C}^1$ anymore). Denote $\partial_x\ell$ the subdifferential of ℓ at x (a set of vectors).

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Let $(\mu,\nu) \in (\mathscr{P}_2(\mathbb{R}^d))^2$, and $\eta \in \Gamma_o(\xi,\nu)$. Integrating the above against η,

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Since η is arbitrary, we obtain that $\xi \in \boldsymbol{\partial}.u(\mu)$.

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Differentiate in length spaces

Def 9 – Metric slope Let (X, d) be a metric space. The metric slope of a map $u : X \to \mathbb{R}$ at the point x is given by

$$|\nabla u(x)| := \overline{\lim_{y \to x}} \frac{|u(y) - u(x)|}{d(x, y)}.$$

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Metric slopes are used to formulate equations in (length) metric spaces, for instance in [AGS05, Vil09, Oht09] on gradient flows, of [GNT08, HK15, GŚ15a, GŚ15b, GHN15] on eikonal-type equations.

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(Last) example: let $u(\mu) = \int_{x \in \mathbb{R}^d} \ell(x) d\mu$ with $\ell \in \mathcal{C}_b^2$. Then $|\nabla^+ u(\mu)| = \int_{x \in \mathbb{R}^d} |\nabla \ell(x)| \, d\mu(x)$.

Gradient flows

In [AGS05], general gradient flows are studied in metric spaces. They want to give a meaning to curves satisfying

$$\frac{d}{dt}y(t) = -\nabla\Phi(y(t)), \qquad y(0) = y_0.$$

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The regular tangent space $\partial.\Phi$ may be two small (case of $\Phi = d^2_{\mathcal{W}}(\cdot,\sigma)$ for instance).

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Eikonal-type equations (HJ depending only on the norm of ∇u)

Canonical example: a minimal time problem

$$-\partial_t u(t,\mu) + \frac{1}{2}\left|\nabla^+ u(t,\mu)\right|^2 = 1, \qquad u(T,\mu) = 0.$$

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The construction of generalized subdifferentials in [AF14] is linked to the tangent cone for curved spaces, explored for the Wasserstein case in [Gig08] (see [AKP22] for material on curved spaces).

The derivatives of the linear map in one glance

Recall that $u : \mathscr{P}_2(\mathbb{R}^d)$ is defined as

$$u(\mu) := \int_{x\in\mathbb{R}^d} \ell(x) d\mu(x).$$

Distributional derivative	Lions derivative	Linear derivative	Natural derivative	Regular subdifferential	General subdifferential
$\text{grad}_\mu u(\mu)$	$\partial_\mu u(\mu)$	$\frac{\delta u}{\delta \mu}(\mu, \cdot)$	$D_\mu u(\mu, \cdot)$	$\partial . u(\mu)$, $\nabla_W u$	$\boldsymbol{\partial} . u(\mu)$
$-\operatorname{div}(\mu \nabla \ell)$	$\nabla \ell$	ℓ	$\nabla \ell$	$\nabla \ell$, select° of $\partial \ell$	$\nabla \ell \# \mu$, $\mathscr{P}(\text{Gr}(\partial \ell))$
distribution, duality with $\mathcal{C}_c^1(\mathbb{R}^d, \mathbb{R})$	element of $L^2_\mu(\mathbb{R}^d, \mathbb{R}^d)$	element of $L^2_\mu(\mathbb{R}^d, \mathbb{R})$	element of $L^2_\mu(\mathbb{R}^d, \mathbb{R}^d)$	element of $T_\mu \mathscr{P}_2(\mathbb{R}^d)$	element of $\boldsymbol{T}_\mu \mathscr{P}_2(\mathbb{R}^d)$

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Open questions:

- How to get out of vector spaces?
- Is there an existence theorem to dig for continuity equations written as $\partial_t \mu_t = -\operatorname{div}(\mu_t F(\mu_t))$, where $F[\mu_t]$ is a plan in $\boldsymbol{T}_\mu \mathscr{P}_2(\mathbb{R}^d)$? Can this be posed pointwise in time, and under which condition does existence hold?

Thank you!

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