

Dissipative evolution of Probability Measures

Giuseppe Savaré Dynamics and Discretization: PDEs, Sampling, and Optimization, October 26, 2021

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Probability vector fields and evolution

Dissipative operators and contraction semigroups in Hilbert spaces

Convergence of the Explicit Euler method and contraction semigroups

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 $\Gamma_o(\mu,\nu):$ optimal couplings for the $L^2\text{-Wasserstein}$ distance. $\gamma_o\in\Gamma_o(\mu,\nu)$ iff

$$W_2^2(\mu,\nu) = \int |x-y|^2 \, d\gamma_o = \min \Big\{ \int |x-y|^2 \, d\gamma : \gamma \in \Gamma(\mu,\nu) \Big\}.$$

Probability vector fields in $\mathcal{P}_2(E)$

Tangent space: $TE = \{(x, v) : x, v \in E\} \approx E \times E$, x(x, v) = x, v(x, v) = v.

In $\mathcal{P}_2(E)$ a probability vector field \mathfrak{F} can be represented by a map (possibly multivalued) from $D(\mathfrak{F})\subset \mathcal{P}_2(E)$ to $\mathcal{P}_2(TE)$ such that

 $\text{for every } \underline{F}\in \mathfrak{F}(\mu): \quad \textbf{x}_{\sharp}\underline{F}=\mu.$

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By disintegrating $\underline{F} \in \mathfrak{F}(\mu)$ w.r.t. μ we obtain a family of measures $F_x \in \mathfrak{P}_2(E)$ which represent probability laws on directions starting from x.

In the "regular case" F_x is concentrated on a single vector $\delta_{\underline{F}(x,\mu)}$ and therefore can be represented by a vector field $\underline{F}(x,\mu)$ mapping $E\times \mathfrak{P}_2(E)$ into E.

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In the general case, we can allow for a general probability measure $F_{\rm x}$ depending on ${\rm x}.$



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$$\dot{\mu}_t = \mathfrak{F}(\mu_t) \quad t > 0.$$

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 \mathfrak{F} does not split particles and it is concentrated on the vector field $\underline{F}(x, \mu)$,

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Examples are

$$\underline{F}(x,\mu) = A(x) + \int B(x-y) \, d\mu(y), \quad A,B:E \to E \text{ dissipative}.$$

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The curve $(\mu_t)_{t>0}$ solves the continuity equation

$$\partial_t \mu_t + \nabla \cdot (\mu_t \boldsymbol{v}_t) = 0, \quad \boldsymbol{v}_t(x) = \underline{F}(x, \mu_t).$$

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Examples

• Gradient flows ² generated by a λ -geodesically convex functional $\mathscr{F}: \mathscr{P}_2(E) \to (-\infty, +\infty]$. \mathscr{F} can be nonsmooth (subdifferential calculus): e.g. ³

$$\mathscr{F}(\mu) = R\Big(\int T(x) \, d\mu(x)\Big) + \iint W(x-y) \, d\mu(x) \, d\mu(y) + \int V \, d\mu$$

$$\begin{split} \mathsf{T}:\mathsf{E}\to\tilde{\mathsf{E}} \text{ is a vector valued map, } \mathsf{R}:\tilde{\mathsf{E}}\to\mathbb{R}, \, W, \, V:\mathsf{E}\to\mathbb{R}.\\ -\mathfrak{F} \text{ is the multivalued Wasserstein subdifferential of } \mathscr{F}. \end{split}$$

²L. AMBROSIO, N. GIGLI, G. S., Gradient flows in metric spaces and in the space of probability measures, Birkäuser, 2008

 $^{^{3}}$ L. CHIZAT, F. BACH, On the global convergence of gradient descent for over-parameterized models using optimal transport, 2018

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 Dissipative evolution, contraction semigroups: E Hilbert space, F multivalued. E.g. the Lipschitz perturbation of a multivalued subgradient. This case has been studied by Piccoli⁴ in finite dimension with a different approach.

 $^{^2}$ L. Ambrosio, N. Gigli, G. S., Gradient flows in metric spaces and in the space of probability measures, Birkäuser, 2008

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This property has a natural metric interpretation: if we consider the curves

$$\mathbf{x}(\tau) := \mathbf{x} + \tau \mathbf{v}, \quad \mathbf{y}(\tau) := \mathbf{y} + \tau \mathbf{w}, \quad \mathbf{v} \in \mathbf{B}\mathbf{x}, \ \mathbf{w} \in \mathbf{B}\mathbf{y}$$

and their squared distance $D(\tau) := \frac{1}{2} |x(\tau) - y(\tau)|^2$

then

$$\langle \nu-w,x-y\rangle=D^{\,\prime}(0)=\frac{1}{2}\frac{d}{d\tau}|x(\tau)-y(\tau)|^2\Big|_{\tau=0}\leqslant 0$$

so that

$$|x(\tau)-y(\tau)|^2 \leqslant |x-y|^2+\tau^2|\nu-w|^2 = |x-y|^2+o(\tau) \quad \text{as } \tau \downarrow 0$$



The resolvent

$$\begin{split} D(\tau) &= \frac{1}{2} |x(\tau) - y(\tau)|^2 \text{ is convex, } D'(0) \leqslant 0 \text{ yields} \\ |x-y|^2 \leqslant |x(s)-y(s)|^2 \quad \text{for every } s < 0 \\ \text{If } x' - \tau B x' &= x \text{ and } y' - \tau B y' = y \\ \text{then } \boxed{|x'-y'|^2 \leqslant |x-y|^2} \end{split}$$



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$$J_\tau := (\mathsf{Id} - \tau B)^{-1}, \quad x' = J_\tau(x) \ \Leftrightarrow \ x' - \tau B x' = x \quad \text{is a contraction}$$

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It follows that for $\tau > 0$ the resolvent

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This property can be used to define dissipative operators in Banach spaces.

B is m-dissipative (or maximal dissipative) if J_{τ} is defined in all the space H: for every $x \in H$ the equation

$$y - \tau By \ni x$$
 has a (unique) solution $y = J_{\tau}x$.

A particular case is the subdifferential $B=-\partial\Phi$ of a convex l.s.c. function $\Phi:H\to(-\infty,+\infty];\ x_\tau=J_\tau(x)$ if and only if

$$x_\tau \text{ minimizes} \qquad y\mapsto \frac{1}{2\tau}|y-x|^2+\Phi(y).$$

If B is everywhere defined, for every $\chi^0_\tau \in H$ one can solve the Explicit Euler method

$$\frac{\mathbf{x}_{\tau}^{n}-\mathbf{x}_{\tau}^{n-1}}{\tau}\in B\mathbf{x}_{\tau}^{n-1}\quad\Leftrightarrow\quad \mathbf{x}_{\tau}^{n}=\mathbf{x}_{\tau}^{n-1}+\tau B\mathbf{x}_{\tau}^{n-1}=(\mathrm{Id}+\tau B)^{n}\mathbf{x}_{\tau}^{0},\quad n=1,\cdots$$

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If B is m-dissipative, for every $x^0_\tau \in H$ one can solve the Implicit Euler method



 $\bar{\mathbf{x}}_{\tau}$ is the piecewise constant interpolant of the values $(\mathbf{x}_{\tau}^{\mathbf{n}})_{\mathbf{n}\in\mathbb{N}}$.

Theorem (Crandall-Liggett '71)

If B is m-accretive, for every $x_0 \in \overline{D(B)}$ the discrete solutions \bar{x}_{τ} of the implicit Eluer scheme converge uniformly to a limit curve $x \in C([0, \infty); H)$.

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Formally

$$\begin{split} &\frac{1}{2}\frac{\mathsf{d}}{\mathsf{d}t}|x(t)-y|^2 = \langle \mathsf{B}x(t),x(t)-y\rangle = \langle \mathsf{B}x(t)-\mathsf{B}y,x(t)-y\rangle + \langle \mathsf{B}y,x(t)-y\rangle \\ &\leqslant \langle \mathsf{B}y,x(t)-y\rangle. \end{split}$$

PVFs and displacement extrapolation

In $\mathcal{P}_2(E)$ the role of the curve $x(\tau) := x + \tau B(x)$ is played by

$$\underline{F}(\tau) := \exp_{\sharp}^{\tau} \underline{F} = (x + \tau \nu)_{\sharp} \underline{F}, \quad \underline{F} \in \mathfrak{F}(\mu).$$

If $(X, V)_{\sharp}\mathbb{P} = \underline{F}$ we have

$$\underline{F}(\tau) = (X + \tau V)_{\sharp} \mathbb{P}$$

Semiconcavity of the Wasserstein distance

If $\underline{F}\in \mathfrak{F}(\mu)$ and $\underline{G}\in \mathfrak{F}(\nu),$ the map

$$D(\tau; \mu, \nu) := \frac{1}{2} W_2^2(\underline{F}(\tau), \underline{G}(\tau))$$

is not convex nor λ -convex for any $\lambda < 0$. In fact it is semiconcave, i.e.

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We can still compute the derivative at $\tau=0$ but

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In particular

The Wasserstein space is Positively Curved (PC)

In $\mathsf{E}=\mathfrak{P}_2(\mathbb{R}^2)$ consider two point masses μ_0 and μ_1 \ldots


































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keeping fixed ν .

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It is usefult to keep in mind that in Hilbert spaces,

$$\frac{d}{dt}\frac{1}{2}\Big|(x+\tau\nu)-y\Big|^2=\langle\nu,x-y\rangle$$

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$$\frac{\mathsf{d}}{\mathsf{d} \mathsf{t}} \frac{1}{2} \Big| (x + \tau \nu) - y \Big|^2 = \langle \nu, x - y \rangle$$

We introduce the set $\Gamma_{\!o}\,(\underline{F},\nu)$ of couplings given by triple of random variables X,V,Y such that

 $(X,V)_{\sharp}\mathbb{P}=\underline{F}, \quad Y_{\sharp}\mathbb{P}=\nu \text{ and }$

 $(X,Y)_{\sharp}\mathbb{P}\in \Gamma_o(\mu,\nu) \text{ is an optimal coupling between } \mu \text{ and } \nu.$

$$[\underline{F},\nu]_{r} = \frac{d}{d\tau} \frac{1}{2} W_{2}^{2}(\underline{F}(\tau),\nu) \Big|_{\tau=0+} = \min \left\{ \mathbb{E} \Big[\langle V, X-Y \rangle \Big] : (X,V,Y) \in \Gamma_{o}(\underline{F},\nu) \right\}$$

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On the other hand

$$[\underline{F},\nu]_{1} = \frac{d}{d\tau} \frac{1}{2} W_{2}^{2}(\mu(\tau),\nu(\tau)) \Big|_{\tau=0-} = \max \Big\{ \mathbb{E} \Big[\langle V, X-Y \rangle \Big] : (X,V,Y) \in \Gamma_{o}(\underline{F},\nu) \Big\}.$$

If
$$v = \dot{x}(0), w = \dot{y}(0)$$

 $\langle v - w, x - y \rangle = \langle v, x - y \rangle + \langle w, y - x \rangle$
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In general

$$[\underline{F},\nu]_{\tau}+[\underline{G},\mu]_{\tau}\leqslant \frac{1}{2}\frac{d}{d\tau}W_{2}^{2}(\underline{F}(\tau),\underline{G}(\tau))\Big|_{\tau=0+}, \qquad \underline{F}\in\mathfrak{F}(\mu), \ \underline{G}\in\mathfrak{F}(\nu).$$

$$\begin{split} f \, \nu &= \dot{x}(0), \, w = \dot{y}(0) \\ & \langle \nu - w, x - y \rangle = \langle \nu, x - y \rangle + \langle w, y - x \rangle \\ &= \frac{d}{d\tau} \frac{1}{2} |x(\tau) - y|^2 \Big|_{\tau = 0} + \frac{d}{d\tau} \frac{1}{2} |y(\tau) - x|^2 \Big|_{\tau = 0} \end{split}$$

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 \mathfrak{F} is (metrically) dissipative if [Cavagnari-Sodini-S.]

 $[\mathfrak{F}(\mu),\nu]_r+[\mathfrak{F}(\nu),\mu]_r\leqslant 0\quad\text{for every }\mu,\nu\in\mathfrak{P}_2(E).$

If $\mathscr{F}: \mathfrak{P}_2(E) \to (-\infty, +\infty]$ is a geodesically convex functional than its (opposite) Wasserstein subdifferential $\mathfrak{F} = -\mathfrak{d}_W \mathscr{F}$ is defined by

 $\underline{F}\in\mathfrak{F}(\mu)\quad\Leftrightarrow\quad [\underline{F},\nu]_{r}\leqslant\mathscr{F}(\nu)-\mathscr{F}(\mu)\quad\text{for every }\nu\in D(\mathscr{F})$

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The Relative Entropy functional

$$\left| \mathscr{F}(\mu) := \int \mathfrak{u}(\log \mathfrak{u} + V) \, \mathsf{d} x = \mathsf{Ent}(\mu|\mathfrak{m}) \quad \text{if } \mu = \mathfrak{u} \mathscr{L}^d \ll \mathscr{L}^d, \quad \mathfrak{m} = \mathsf{e}^{-V} \mathscr{L}^d.$$

 $\mathscr{F} \equiv +\infty$ on the discrete measures. \mathscr{F} is geodesically convex (i.e. convex along displacement interpolations, [McCann '97]) but not convex along arbitrary interpolation of measures: optimal interpolations avoid collisions!

If <u>F</u> arises as the gradient of a displacement convex functional \mathscr{F} , we can also use a variational formulation of the implicit Euler method.

⁵R. JORDAN, D. KINDERLEHRER, F. OTTO, The variational formulation of the Fokker-Planck equation. SIAM J. Math. Anal. (1998) L. AMBROSIO, N. GIGLI, G. S. (2008),

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According to the JKO -Minimizing Movement approach ⁵, at each step it is sufficient to select μ_{τ}^{n} among the minimizers of

$$\mu\mapsto \frac{1}{2\tau}W_2^2(\mu, \boldsymbol{\mu_\tau^{n-1}})+\mathscr{F}(\mu)$$

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Wasserstein gradient flows

Let $\mathscr{F}: \mathfrak{P}_2(E) \to (-\infty, +\infty]$ be a lower semicontinuous and displacement convex functional. We say that a locally Lipschitz curve $(\mu_t)_{t>0}$ is an EVI-solution of the gradient flow of \mathscr{F} if for every $\nu \in D(\mathscr{F}) \subset \mathfrak{P}_2(E)$

$$\frac{d}{dt}\frac{1}{2}W_2^2(\mu_t,\nu)\leqslant \mathscr{F}(\nu)-\mathscr{F}(\mu_t) \quad \text{a.e. in } (0,\infty)$$

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(EVI)

Theorem (Ambrosio-Gigli-S.)

For every initial datum $\mu_0 \in \overline{D(\mathscr{F})}$ there exists a unique EVI solution to (EVI) satisfying $\lim_{t\downarrow 0} \mu_t = \mu_0$.

Moreover, μ is the uniform limit of piecewise constant interpolant μ_{τ} of the JKO-Minimizing Movement approximations, obtained by solving

$$\mu^n_{\pmb{\tau}} \in \underset{\mu}{\text{argmin}} \left\{ \frac{1}{2\tau} W_2^2(\mu, \mu^{n-1}_{\pmb{\tau}}) + \mathscr{F}(\mu) \right\}, \quad \mu^0_{\pmb{\tau}} := \mu_0$$

Uniform error estimate if $\mu_0\in D(\mathscr{F})$:

 $W_2(\mu(t), \mu_{\tau}(t)) \leqslant C\sqrt{\tau}.$

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- Technical point: perturbations along \mathfrak{F} can split particles.
- \mathfrak{F} behaves well only along (optimal) displacement interpolations.

Probability vector fields and evolution

Dissipative operators and contraction semigroups in Hilbert spaces

Convergence of the Explicit Euler method and contraction semigroups

The explicit Euler method for dissipative evoutions

We can construct solutions to the evolution equation by means of the Explicit Euler method:

we fix a step size $\tau > 0$, an initial measure μ_0 . If \mathfrak{F} is a dissipative vector field and $\tau > 0$ is a time step, we consider the curves $\underline{F}(\tau)$ in $\mathfrak{P}_2(E)$, $\underline{F} \in \mathfrak{F}(\mu)$

$$\underline{F}(\tau) := exp_{\sharp}^{\tau} \, \underline{F} = (x + \tau \nu)_{\sharp} \underline{F}, \quad \underline{F} \in \mathfrak{F}(\mu)$$

and therefore the sequence of explicit Euler approximations:

$$\mu^0_\tau \coloneqq \mu_0 \text{ given}, \quad \mu^{n+1}_\tau \coloneqq \underline{F}^n(\tau), \ \underline{F}^n \in \mathfrak{F}(\mu^n_\tau), \quad \mu_\tau(t) \coloneqq \mu^{\lfloor t/\tau \rfloor}_\tau$$

 μ_{τ} is the piecewise constant interpolation, $\mu_{\tau}(t) = \mu_{\tau}^{n}$ if $n\tau \leq t < (n+1)\tau$.

Problems: convergence of the method and characterization of the limit.

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Problems: convergence of the method and characterization of the limit.

Easy "Lipschitz" estimate:

$$\frac{W_2(\boldsymbol{\mu}^{\mathbf{n}}_{\boldsymbol{\tau}}, \boldsymbol{\mu}^{\mathbf{n}-1}_{\boldsymbol{\tau}})}{\tau} \leqslant \Big(\int |\nu|^2 \, \mathsf{d}\underline{F}^{\mathbf{n}}(\boldsymbol{x}, \nu)\Big)^{1/2}$$

 $\mathscr{M}(\mu_0, \tau, L, T)$:= set of discrete solutions μ_{τ} of the Explicit Euler method starting from μ_0 , defined up to the final time T, such that

$$\int |\nu|^2\,d\underline{F}^n(x,\nu)\leqslant L^2\quad\text{for every }n\leqslant \lfloor T/\tau\rfloor.$$

Theorem (Cavagnari-Sodini-S.)

Suppose that \mathfrak{F} is a dissipative MPVF.

• If $k \mapsto \tau(k) \downarrow 0$ is a vanishing sequence of step sizes and $\mu_{k} \in \mathscr{M}(\mu_{0}, \tau(k), L, T)$ for some $L \ge 0$, then the sequence of discrete solutions μ_{k} of the explicit Euler method uniformly converge to a unique limit $\mu : [0, T] \rightarrow \mathcal{P}_{2}(E)$.

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- μ is a Lipschitz curve and it is the unique solution of the disspative EVI (in the distributional sense of D'(0, T))

 $|\frac{d}{dt}\frac{1}{2}W_2^2(\mu(t),\nu)\leqslant -[F(\nu),\mu]_{\mathrm{r}}\quad \text{for every }\nu\in D(\mathfrak{F});\quad \mu(0)=\mu_0,$
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• We have the optimal error estimate

 $W_2(\mu(t), \boldsymbol{\mu_\tau(t)}) \leqslant CL\sqrt{T\tau} \quad \textit{for every } t \in [0,T].$

Generation of a flow of contractions

Suppose that \mathfrak{F} is a dissipative MPVF such that $D(\mathfrak{F})$ contains all the measures with bounded support of $\mathfrak{P}_{\mathfrak{b}}(\mathsf{E}).$

Suppose moreover that

• for every $\mu_0\in \mathfrak{P}_b(E)$ there exist $\rho,L>0$ such that

 $W_2(\mu,\mu_0) < \rho \quad \Rightarrow \quad \exists \, \underline{F} \in \mathfrak{F}(\mu): \text{supp}(\nu_\sharp \underline{F}) \subset B_L(0).$

(local solvability of the Explicit Euler method)

- every $\underline{F}\in\mathfrak{F}$ is concentrated on the set

 $(\mathbf{x}, \mathbf{v}) \in \mathbf{E} \times \mathbf{E}$: $\langle \mathbf{v}, \mathbf{x} \rangle \leqslant \mathbf{C}(1 + |\mathbf{x}|^2)$

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Theorem

Then \mathfrak{F} generates a semigroup of contractions: for every $\mu_0 \in \mathfrak{P}_2(E)$ there exists a unique continuous curve $\mu = S[\mu_0] \in C([0,\infty); \mathfrak{P}_2(E))$ such that

 $\left|\frac{d}{dt}\frac{1}{2}W_2^2(\mu(t),\nu)\leqslant -[F(\nu),\mu]_{\mathfrak{r}}\quad \textit{for every }\nu\in D(\mathfrak{F})\quad \mu(0)=\mu_0,$

 $W_2(\boldsymbol{S}_t[\mu_0], \boldsymbol{S}_t[\nu_0]) \leqslant W_2(\mu_0, \nu_0) \quad \textit{for every } \mu_0, \nu_0 \in \mathcal{P}_2(E), \ t > 0.$

Barycentric property

Under the same conditions, let us also suppose that the sections $\mathfrak{F}(\mu)$ of \mathfrak{F} are convex and the graph of \mathfrak{F} is closed under strong-weak convergence: if a sequence $\underline{F}_n \in \mathfrak{F}(\mu_n)$ satisfies

$$\label{eq:matrix} \begin{split} \mu_n \to \mu \text{ in } \mathcal{P}_2(E), \quad \underline{F}_n \to \underline{F} \text{ in } \mathcal{P}(E \times E), \quad \sup_n \int |\nu|^2 \, d\underline{F}_n(x,\nu) < \infty \end{split}$$
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then $\underline{F} \in \mathfrak{F}(\mu)$.

Theorem

Every EVI solution $\mu:(0,\infty)\to D(\mathfrak{F})$ satisfies the barycentric property: for $\mathscr{L}^1\text{-}a.e.\ t>0$ there exists $\underline{F}_t\in\mathfrak{F}(\mu_t)$ such that

$$\frac{d}{dt} \int \zeta(x) \, d\mu_t(x) = \int \langle D\zeta(x), \nu \rangle \, d\underline{F}_t(x, \nu) \tag{(*)}$$

for every smooth bounded Lipschitz cylindrical function $\zeta : E \to \mathbb{R}$.

Conversely, if $\mu:(0,\infty)\to D(\mathfrak{F})$ is absolutely continuous, it satisfies (\star) , and for a.e. t>0 $\mu_t\in \mathfrak{P}_2^r(E)$ or $\mathfrak{F}(\mu_t)$ contains a unique element concentrated on a map, μ is also an EVI solution.

 $(\star) \text{ is equivalent to } \qquad \partial_t \mu_t + \nabla \cdot (\mu_t \nu_t) = 0, \quad \nu_t = proj_{\mathsf{Tan}(\mu_t)}(\underline{F}_t)$

- Everything can be easily extended to λ -dissipative probability vector fields.
- Evolutions do not split particles in dimension $\ge 2?$
- $\bullet\,$ Impose only local boundedness on $\mathfrak F$
- Implicit Euler scheme
- Stability and G-convergence
- ...