W_2 gradient flows and PDE

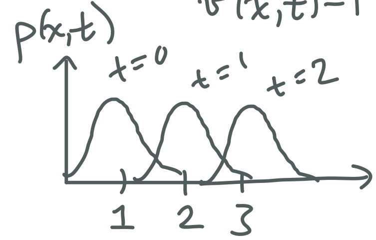
$d\rho(x) = \rho(x)\,dx$

Motivation: $\rho(x,t) \geq 0$, $\int \rho(x,t)\,dx = 1$

$x_1(t), \dots, x_n(t) \in \mathbb{R}^d$

⓪ Continuity equation

$v(x,t) = 1$



PDE: $\begin{cases} \partial_t \rho + \nabla \cdot (v\rho) = 0 \\ \rho(x,0) = \rho_0(x) \end{cases}$

$t \in [0,T]$

Particles: $\begin{cases} \dot{x}_i(t) = v(x_i(t), t) \\ x_i(0) = x_{i,0} \end{cases}$ $\quad W_2(\rho^N(t), \rho(t)) \leq C_{T, \|\nabla v\|_\infty} W_2(\rho^N(0), \rho(0))$

$$\boxed{\begin{array}{l} \text{For } v \text{ nice, if } \rho^N(0) = \frac{1}{N}\sum_{i=1}^N \delta_{x_{i,0}} \xrightarrow{N \to +\infty} \rho_0(x), \\ \text{then } \rho^N(t) = \frac{1}{N}\sum_{i=1}^N \delta_{x_i(t)} \xrightarrow{N \to +\infty} \rho(x,t). \end{array}}$$

① Aggregation eqn w/ drift [AGS'05, CDFLS'10]

$v(x)$ $\quad W(x) = \pm \frac{|x|^{2-d}}{2-d}$, $\frac{|x|^a}{a} - \frac{x^b}{b}$, $-d < b \leq a$

PDE: $\partial_t \rho = \nabla \cdot (\nabla V \rho) + \nabla \cdot ((\nabla W * \rho)\rho)$

Particles: $\dot{x}_i(t) = -\nabla V(x_i(t)) - \frac{1}{N}\sum_{j=1}^N \nabla W(x_i(t) - x_j(t))$

Energy: $E(\rho) = \int V(x)\rho(x)\,dx + \frac{1}{2}\iint W(x-y)\rho(x)\rho(y)\,dx\,dy$

② Fokker–Planck eqn:

$\partial_t \rho + \nabla\cdot(\underbrace{(-\nabla V) + (-\tfrac{\nabla \rho}{\rho})}_{v(x,t)}\rho) = 0$

PDE: $\partial_t \rho = \nabla\cdot(\nabla V \rho) + \Delta \rho$

Particles: $dX_t = \sqrt{2}\, dB_t - \nabla V(X_t)\,dt$

Energy: $E(\rho) = \int V(x)\rho(x)\,dx + \int \rho(x)\log\rho(x)\,dx$

③ 2-layer NN: [MMN'18], [RVE'18], [CB'18], ..

$\Phi(x,z) = x_i\left(\sum_i x_i z_i + x_d\right)_+$

$\Phi(x,z) = \psi(|x-z|)$

Energy: $E(\rho) = \frac{1}{2}\int \left|\int \Phi(x,z)\rho(x)\,dx - f_0(z)\right|^2 d\nu(z)$

$$= \frac{1}{2}\iint \overbrace{\int \Phi(x,z)\Phi(y,z)\,d\nu(z)}^{\omega(x,y)}\, \rho(x)\rho(y)\,dx\,dy$$

$$- \int \underbrace{\int \Phi(x,z) f_0(z)\,d\nu(z)}_{V(x)}\, \rho(x)\,dx + C$$

④ Blob method for χ^2 GF [CLLMR, '20], [CEHT, in prep]

Energy: $E(\rho) = \frac{1}{2}\int \frac{|\rho(x) - \bar\rho(x)|^2}{\bar\rho(x)}\,dx$

Another energy: $E_\varepsilon(\rho) = \frac{1}{2}\int \frac{|\varphi_\varepsilon * \rho(x) - \bar\rho(x)|^2}{\bar\rho(x)}\,dx$

Moral: W_2 perspective brings new tools that complement pure PDE/particle pespective

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Plan

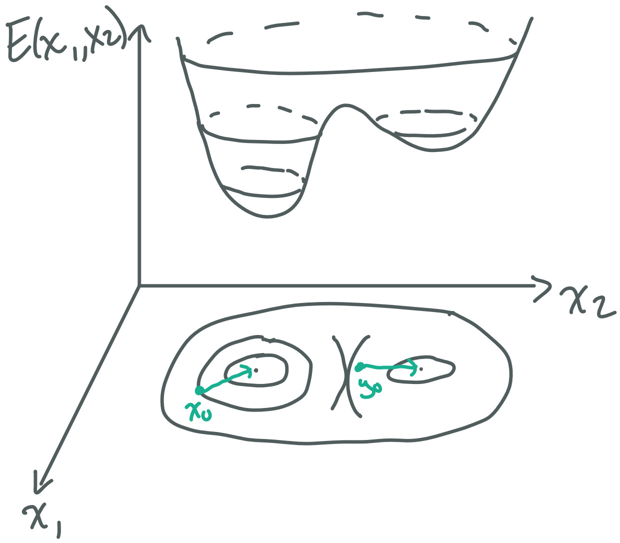
1) Warmup: GF on $\mathbb{R}^d$
2) GF and PDE
3) GF on metric spaces
4) Wasserstein GF

Warmup: GF on $\mathbb{R}^d$

Consider $E: \mathbb{R}^d \to \mathbb{R}$, $x_0 \in \mathbb{R}^d$.

Def: A gradient flow of E with initial conditions x_0 is a solution of

$$\begin{cases} \dot{x}(t) = -\nabla E(x(t)), & t \geq 0 \\ x(0) = x_0 \end{cases}$$



EXISTENCE

- $E \in C^1(\mathbb{R}^d)$ (at least for short time)

UNIQUENESS/ $t \to +\infty$

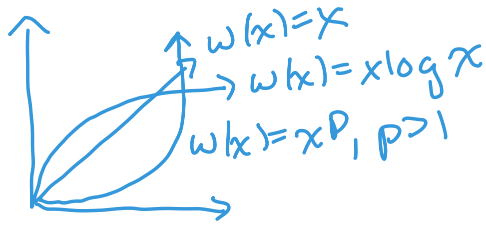
- one sided Lipschitz: $\exists\ \lambda \in \mathbb{R}$ s.t.

$$\langle x-y, \nabla E(x) - \nabla E(y) \rangle \geq \lambda |x-y|^2, \quad \forall\, x,y \in \mathbb{R}^d$$

$E \in C^1$

- above tangent line ineq: $\exists\, \lambda \in \mathbb{R}$ s.t.
  $$E(y) - E(x) - \langle \nabla E(x), y-x \rangle \geq \frac{\lambda}{2}|x-y|^2 \quad \forall x,y \in \mathbb{R}^d$$
  for $\omega(x)$ cts, increasing, $\omega(0)=0$ $\qquad \frac{\lambda}{2}\omega(|x-y|)^2$

- λ-convex: $\exists\, \lambda \in \mathbb{R}$ s.t.
  $$E((1-\alpha)x + \alpha y) \leq (1-\alpha)E(x) + \alpha E(y) - (1-\alpha)\alpha \frac{\lambda}{2}|x-y|^2 \quad \forall x,y \in \mathbb{R}^d,\ \alpha \in [0,1]$$



Why does this imply uniqueness?

Suppose $x(t)$ and $y(t)$ are gradient flows of E.

$$\frac{d}{dt}|x(t)-y(t)|^2 = 2\langle x(t)-y(t), -\nabla E(x(t)) + \nabla E(y(t))\rangle$$
$$\leq -2\lambda |x(t)-y(t)|^2$$

$$|x(t)-y(t)|^{\cancel{2}} \leq e^{-\cancel{2}\lambda t}|x(0)-y(0)|^{\cancel{2}}, \quad t \geq 0$$

$$\frac{d}{dt}a(t) = -2\lambda a(t)$$
$$a(t) = a(0)e^{-2\lambda t}$$

$w(x) = x\log x \qquad \text{RHS} = |x(0)-y(0)|^{e^{2\lambda t}}$

$w(x) = x^p,\ p>1 \qquad \text{RHS} = \left((p-1)2\lambda t + |x(0)-y(0)|^{2(1-p)}\right)^{\frac{1}{2(1-p)}}$

Rmk:

- $\overset{E\in C^2}{\Longleftrightarrow} D^2E \geq \lambda I_{d\times d}$
- E_0 is λ_0-convex, E_1 is λ_1-convex, then E_0+E_1 is $(\lambda_0+\lambda_1)$-convex
- $\lambda>0 \Rightarrow E$ is strongly convex
- $(1-\alpha)x+\alpha y$ is the geodesic from x to y

GENERALIZE TO METRIC SPACE?

Energy dissipation equality (EDE)

$$\dot{x}(t) = -\nabla E(x(t)) \Longleftrightarrow \begin{array}{l} |\dot{x}(t)| = |\nabla E(x(t))| \\ \frac{d}{dt}E(x(t)) = -|\nabla E(x(t))|\,|\dot{x}(t)| \end{array}$$

$ab \geq -\frac{a^2}{2} - \frac{b^2}{2}$ with "=" only if $a=-b$

$$\Longleftrightarrow \frac{d}{dt}E(x(t)) \leq -\frac{1}{2}|\nabla E(x(t))|^2 - \frac{1}{2}|\dot{x}(t)|^2$$

Time discretization

Suppose E lower semicts, λ-convex.

$$\begin{cases} \dot{x}(t) = -\nabla E(x(t)) \\ x(0) = x_0 \end{cases} \xrightarrow[\text{Euler}]{\text{Implicit}} \begin{array}{l} \frac{x_n - x_{n-1}}{\tau} = -\nabla E(x_n) \quad n\geq 1 \\ x_0 = x_0 \end{array}$$

Given x_{n-1},

$$x_n = \underset{x}{\operatorname{argmin}} \left\{ \underbrace{\overbrace{\frac{1}{2\tau}|x - x_{n-1}|^2}^{\frac{1}{\tau}\text{ convex}} + \overbrace{E(x)}^{\lambda\text{convex}}}_{\frac{1}{\tau}+\lambda \text{ convex}} \right\}$$ "Proximal map"

- energy dissipation: $$\frac{E(x_n) - E(x_{n-1})}{\tau} \leq \frac{-1}{2\tau^2} |x_n - x_{n-1}|^2$$

$$\xrightarrow{\tau = \frac{t}{n},\ n \to +\infty} e^{-\lambda t}$$

- contraction: $$|x_n - y_n| \leq \left(\frac{1}{1+\lambda\tau}\right)^{n-1} |x_0 - y_0|$$

GF and PDE

Ex:

metric	$(L^2(\mathbb{R}^d), \|\cdot\|_{L^2})$	$(\mathcal{P}_2(\mathbb{R}^d), W_2)$
gradient	$\nabla_{L^2} E(f) = \frac{\delta E}{\delta f}$	$\nabla_{W_2} E(\rho) = -\nabla\cdot\left(\rho \nabla \frac{\delta E}{\delta \rho}\right)$
energy	$E(f) = \frac{1}{2}\int \|\nabla f\|^2$	$E(\rho) = \frac{1}{m-1}\int \rho^m + \int V\rho + \frac{1}{2}\int (W * \rho)\rho$ $m=1 \rightarrow \int \rho\log\rho$
GF	$\partial_t f = \Delta f$	$\partial_t \rho = \Delta \rho^m + \nabla\cdot((\nabla V + \nabla W * \rho)\rho)$

GF structure helps with $E(\rho) = \int V\rho$

GF on metric spaces

(X, d) complete metric space

What is analogue of $\dot{x}(t) = -\nabla E(x(t))$?

$$\Updownarrow \ \mathbb{R}^d$$

$$\frac{d}{dt} E(x(t)) \leq -\frac{1}{2}|\nabla E(x(t))|^2 - \frac{1}{2}|\dot{x}(t)|^2$$

Consider $x : [0,T] \to X$, $E : X \to \mathbb{R} \cup \{+\infty\}$

- metric derivative: $|x'|(t) = \lim_{s \to t} \frac{d(x(s), x(t))}{|s-t|}$

  $s_+ = \max\{0, s\}$

- metric slope: $|\partial E|(x) = \limsup_{y \to x} \frac{(E(x) - E(y))_+}{d(x,y)}$
- $x \in AC^2([0,T], X)$ in case $|x'|(t) \in L^2([0,T])$.

Def: $x \in AC^2([0,T], X)$ is the curve of maximal slope of E with initial data x_0 if $x(0) = x_0$ and

$$E(x(t)) - E(x(s)) \leq -\frac{1}{2}\int_s^t |\partial E|^2(x(r))\,dr - \frac{1}{2}\int_s^t |x'|^2(r)\,dr$$

energy decreasing

$\forall\ 0 < s \leq t \leq T$

Questions

- existence?
- uniqueness?
- key properties?
- coincide w/ W_2-GF for $(X,d) = (\mathcal{P}_2(\mathbb{R}^d), W_2)$?

Def: $x:[0,1] \to X$ is a *geodesic* if
$d(x(\alpha), x(\beta)) = |\alpha - \beta| \, d(x(0), x(1))$.

Def: $E: X \to \mathbb{R} \cup \{+\infty\}$ is *λ-convex* if $\forall\, x_0, x_1 \in X$ $\exists$ geodesic $x(\alpha)$ from x_0 to x_1 s.t. $\forall\, \alpha \in [0,1]$,

$$E(x(\alpha)) \leq (1-\alpha) E(x(0)) + \alpha E(x(1)) - (1-\alpha)\alpha \frac{\lambda}{2} d(x_0, x_1)^2$$

$\boxed{\text{TIME DISCRETIZATION}}$

Given x_{n-1},

$$x_n = \underset{x}{\operatorname{argmin}} \Big\{ \underbrace{\frac{1}{2\tau} d(x, x_{n-1})^2 + E(x)}_{\Phi_{x_{n-1}}(x)} \Big\}$$

"Minimizing Movements" [DG, '93], "JKO" [JKO, '98]

Well-defined?

Non-positive curvature metric space

- if $x \mapsto \frac{1}{2} d(x, x_0)^2$ is 1-convex $\forall\, x_0 \in X$, then E λ-convex is sufficient.
- what about if $x \mapsto \frac{1}{2} d(x, x_0)^2$ is nonconvex?

it is λ-convex and

$\swarrow$ λ-cgg

<u>Def</u>: $E: X \to \mathbb{R} \cup \{+\infty\}$ is <u>λ-convex along generalized geodesics</u> if $\forall x_0, x_1, \tilde{x}$, $\exists$ a curve $x(t)$ from x_0 to x_1 s.t. $\Phi_{\tilde{x}}(x)$ is $(\frac{1}{\tau}+\lambda)$-convex for $\frac{1}{\tau}+\lambda > 0$.

$D(E) = \{x : E(x) < +\infty\}$

<u>Thm</u> <u>(AGS'05)</u> If E is lsc and λ-cgg, $\forall x_0 \in D(E)$, $\exists !$ curve of max slope. Also

- EDE, $\frac{d}{dt} E(x(t))$ exists
- $d(x(t), y(t)) \leq e^{-\lambda t} d(x(0), y(0))$
- time discretization converges $O(\tau)$.

Wasserstein GF

$(\mathcal{P}_2(\mathbb{R}^d), W_2)$

How does a curve of max slope relate to PDE?

Three key properties of W_2: [AGS'05]

① if $\rho \in AC^2([0,1], \mathcal{P}_2(\mathbb{R}^d))$, $\exists\, v(x,t)$ s.t. $\partial_t \rho + \nabla \cdot (v \rho) = 0$ and $\left(\int |v(x,t)|^2 \rho(x,t)\, dx\right)^{1/2} = |\rho'|(t)$

PDE Benamou-Brenier for a.e. t

Suppose E is lsc and λ-cgg.

pseudo-Riemannian structure gives chain rule.

(2) For $\xi \in \partial E(\rho(t))$, $\frac{d}{dt} E(\rho(t)) = \int \langle \xi(x), v(x,t) \rangle \rho(x,t)\, dx$

Suppose $\frac{\delta E}{\delta \rho}$ is "well-defined".

(3) $\nabla \frac{\delta E}{\delta \rho} \in \partial E(\rho)$ and $|\partial E|(\rho) = \left(\int |\nabla \frac{\delta E}{\delta \rho}|^2 d\rho \right)^{1/2}$

Nice expression

Then...

Thm [AGS'05] If $\rho(x,t)$ is the curve of max slope of E, then $\partial_t \rho - \nabla \cdot (\nabla \frac{\delta E}{\delta \rho} \rho) = 0$.

Pf: By (1), there exists $v(x,t)$ s.t. $\partial_t \rho + \nabla \cdot (v\rho) = 0$. Thus it suffices to show $v = -\nabla \frac{\delta E}{\delta \rho}$.

$$\frac{d}{dt} E(\rho(t)) = \int \langle \underbrace{\xi(x)}_{\overset{(3)}{=}\nabla \frac{\delta E}{\delta \rho}}, v(x,t) \rangle \rho(x,t)\, dx$$

$ab \geq -\frac{a^2}{2} - \frac{b^2}{2}$ with "=" only if $a = -b$

$$\geq -\frac{1}{2} \|\nabla \frac{\delta E}{\delta \rho}\|^2_{L^2(\rho)} - \frac{1}{2} \|v\|^2_{L^2(\rho)}$$

$$= -\frac{1}{2} |\partial E|^2(\rho(t)) - |\rho'|^2(t)$$

$$\geq \frac{d}{dt} E(\rho(t)).$$

Thus $v = -\nabla \frac{\delta E}{\delta \rho}$, ρ-a.e. $\square$

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