FOKKER-PLANCK AS A WASSERSTEIN GRADIENT FLOW

GRADIENT FLOWS IN METRIC SPACES

(X, d) $\quad F : X \to \overline{\mathbb{R}}$

$F : \mathbb{R}^n \to \mathbb{R}$

NO MEANING IN A METRIC SETTING

$$\begin{cases} x'(t) = -\nabla F(x(t)) \\ x(0) = x_0 \end{cases}$$

TIME-DISCRETIZATION: FIX $\tau > 0$

$$x_{k+1} \in \operatorname{argmin} \; F(x) + \frac{|x - x_k|^2}{2\tau}$$

$$\nabla F(x) + \frac{x - x_k}{\tau} = 0 \qquad x = x_{k+1}$$

$$\min \; F(x) + \frac{d(x, x_k)^2}{2\tau}$$

$$\frac{x_{k+1} - x_k}{\tau} = -\nabla F(x_{k+1})$$

IMPLICIT EULER SCHEME

FULL ABSTRACT THEORY: AMBROSIO, GIGLI, SAVARÉ

WE'LL USE $X = \mathcal{P}(\Omega)$ $\Omega \subset \mathbb{R}^d$ COMPACT

= PROBABILITIES ON Ω

$d = W_2$ WASSERSTEIN DISTANCE, COMING FROM OT.

$c : \Omega \times \Omega \to \mathbb{R}$ $\mu, \nu \in \mathcal{P}(\Omega)$

OT

$$\min \left\{ \int_{\Omega \times \Omega} c \, d\gamma \ : \ \begin{array}{l} \gamma \in \mathcal{P}(\Omega \times \Omega) \\ \pi_x \# \gamma = \mu \quad \pi_y \# \gamma = \nu \end{array} \right\}$$

IF I USE $c(x,y) = |x-y|^p$ $1 \leq p < +\infty$

$$W_p(\mu, \nu) = \left(\min \left\{ \int c \, d\gamma \ \ldots \right\} \right)^{1/p}$$

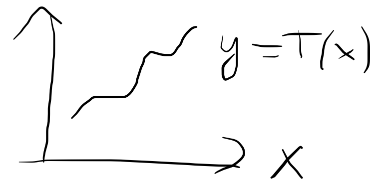
THIS IS A DISTANCE ON $\mathcal{P}(\Omega)$ CALLED WASSERSTEIN DISTANCE

$$W_p(\mu_n, \mu) \to 0 \iff \mu_n \xrightarrow{*} \mu$$

$$\frac{1}{2} W_2^2(\mu, \nu) = \min \int \frac{1}{2} |x-y|^2 \, d\gamma \quad \ldots \qquad \text{KANTOROVICH}$$

$$= \min \left\{ \int \frac{1}{2} |x - T(x)|^2 \, d\mu \quad \left. \begin{array}{l} T : \Omega \to \Omega \\ T_{\#}\mu = \nu \end{array} \right\} \right. \qquad \text{MONGE}$$

(THE OPTIMAL γ IS OF THE FORM $(id, T)_{\#}\mu$)



$$= \sup \left\{ \int \varphi \, d\mu + \int \psi \, d\nu \; : \; \begin{array}{l} \varphi, \psi \in C^0(\Omega) \\ \varphi(x) + \psi(y) \le \frac{1}{2}|x-y|^2 \end{array} \right\}$$

(DUAL FORMULATION OF OT)

FACTS ON T, φ, ψ :

- $T(x) = x - \nabla\varphi(x) = \nabla\left(\frac{|x|^2}{2} - \varphi\right) = \nabla$ CONVEX
- φ IS LIP
- $\varphi(x) = \inf_y \frac{1}{2}|x-y|^2 - \psi(y)$

$$\Rightarrow \varphi(x) - \frac{1}{2}|x|^2 = \inf_y -x\cdot y + \frac{1}{2}|y|^2 - \psi(y)$$

$= \inf$ AFFINE

$=$ CONCAVE

$\Rightarrow D^2\varphi \leq I$

- $T_\# \mu = \nu$ IF μ, ν HAVE DENSITIES

$DT = I - D^2\varphi \geq 0$

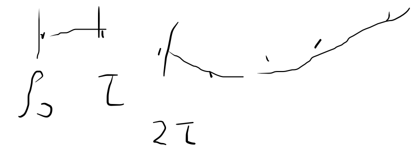
$$\mu(x) = \nu(T(x))|\det DT(x)|$$
$$= \nu(x - \nabla\varphi(x)) \det(I - D^2\varphi)$$

MONGE-AMPÈRE

- CAFFARELLI'S REGULARITY ! Ω CONVEX μ, ν NICE $\Rightarrow$ φ, T SMOOTH

GRADIENT FLOWS IN W_2

$$F : \mathcal{P}(\Omega) \longrightarrow \overline{\mathbb{R}}$$



$$\min \; F(\rho) + \frac{W_2^2(\rho, \rho_k)}{2\tau}$$

NOTATION: I call $\frac{\delta F}{\delta \rho}$ ANY FUNCTION S.T.
$$\frac{d}{d\varepsilon} F\big(\overbrace{\underset{\in \mathcal{P}(\Omega)}{\rho} + \varepsilon \chi}^{\in \mathcal{P}(\Omega)}\big)\Big|_{\varepsilon=0} = \int \frac{\delta F}{\delta \rho}\, d\chi$$

(IF IT EXISTS; IN THIS CASE IT IS DEFINED UP TO ADDITIVE CONSTS. SINCE $\int d\chi = 0$)

$$\frac{\delta F}{\delta \rho} + \frac{1}{\tau} \frac{\delta \, \frac{1}{2} W_2^2(\cdot, \rho_k)}{\delta \rho} = C$$

EXAMPLES

$$F(\rho) = \int V \, d\rho \Rightarrow \frac{\delta F}{\delta \rho} = V$$

$$F(\rho) = \int f(\rho(x))\,dx \Rightarrow \frac{\delta F}{\delta \rho} = f'(\rho)$$

$$F(\rho) = \frac{1}{2} W_2^2(\rho, \nu) \Rightarrow \frac{\delta F}{\delta \rho} = \varphi$$ (THE OPTIMAL φ IN THE DUAL OT)

$\rightarrow x - T(x)$

$$\nabla \frac{\delta F}{\delta \rho} + \frac{\nabla \varphi}{\tau} = \text{CONST}$$

POSITION AT STEP $k+1$

POSITION AT STEP k

$$\underbrace{\frac{x - T(x)}{\tau}}_{v(x) \,=\, \text{VELOCITY}} = -\nabla \frac{\delta F}{\delta \rho}$$

$$T_{\#} \rho_{k+1} = \rho_k$$

"AT THE LIMIT $\tau \to 0$" ρ WILL BE A CURVE OF DENSITIES

$$\partial_t \rho + \nabla \cdot (\rho v) = 0$$ ρ IS ADVECTED BY $v = -\nabla \frac{\delta F}{\delta \rho}$

A PARABOLIC PDE !!

IF $F(\rho) = \int f(\rho(x))\,dx + \int V\,d\rho$

$-\nabla\cdot(\rho\nabla V)$

$$\partial_t \rho - \nabla\cdot\left(\rho\nabla\left(f'(\rho)\right)\right) = 0$$

NONLINEAR DIFFUSION EQ

IF $f(s) = s\log s$ $\quad f'(s) = \log s + 1$ $\quad \nabla f'(\rho) = \dfrac{\nabla\rho}{\rho}$

$$\partial_t \rho - \Delta\rho - \nabla\cdot(\rho\nabla V) = 0$$

FOKKER-PLANCK EQN.

$$F(\rho) = \int \rho\log\rho + \rho V$$

WE CAN OBTAIN THIS PDE BY LOOKING AT

$$\min \int \rho\log\rho + \rho V + \frac{1}{2\tau} W_2^2(\rho, g)$$

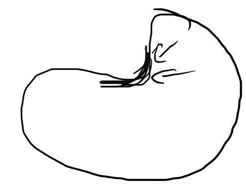
$g = \rho_k$

QUESTIONS: WHICH BOUNDS ON g PASS TO THE OPTIMAL ρ?

FOR INSTANCE (UNDER SOME ASSUMPTIONS) IF $a \le \log g + V \le b$

$\Longrightarrow a \le \log \rho + V \le b$ SAME BOUNDS!!

HOW TO PROVE THIS $\boxed{L^\infty \text{ BOUND}}$



TAKE $x \in \mathring{\Omega}$ a max point for $\log \rho + V$

$$\underbrace{\frac{\delta F}{\delta \rho}}_{=\,\log \rho + V} + \frac{\varphi}{\tau} = c \quad \Longrightarrow \quad \varphi \text{ is min} \quad \Longrightarrow \quad \nabla \varphi(x) = 0, \quad I \geq D^2 \varphi(x) \geq 0$$

$$\rho(x) = g(T(x)) |\det DT(x)| =$$

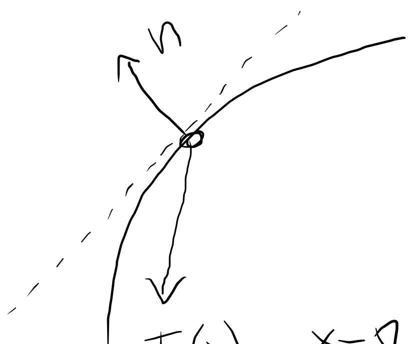
$$= g(x - \underbrace{\nabla \varphi(x)}_{=\,0}) \det(\underbrace{I - D^2 \varphi(x)}_{\leq I}) \leq g(x)$$

$$\log \rho(x) + V(x) \leq \log g(x) + V(x) \leq b \quad \Longrightarrow \quad \log \rho + V \leq b$$

SAME FOR min $\log \rho + V$

DIFFICULTY: IF $x \in \partial\Omega$. IF $\Omega = \mathbb{T}^d$ TORUS IT'S OK

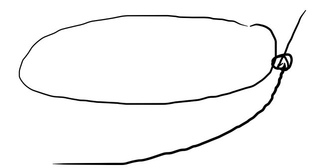
IF Ω CONVEX x MAX POINT FOR $\log \rho + V \Rightarrow$ min FOR φ



$T(x) = x - \nabla\varphi(x)$

$$(x - \nabla\varphi(x)) \cdot n \le x \cdot n$$

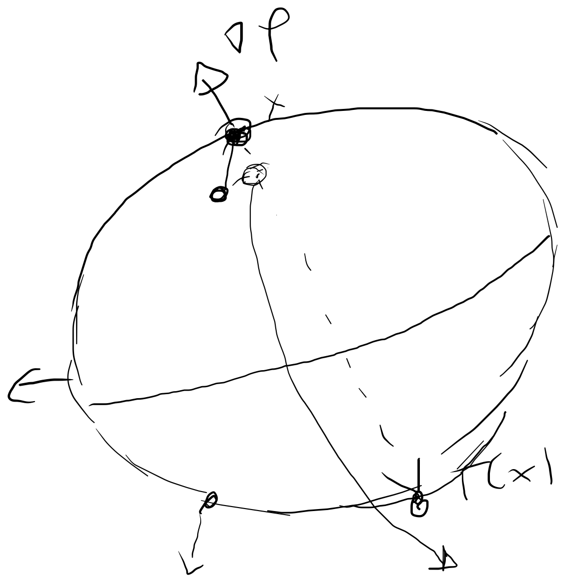
$$\Rightarrow \frac{\partial \varphi}{\partial n} \ge 0$$



$\Rightarrow$ CONTRADICTION (UNLESS $\frac{\partial \varphi}{\partial n} = 0 \Rightarrow \nabla\varphi = 0$

$\Rightarrow D^2\varphi \ge 0$ . . . .)

IF x IS A MIN FOR $\log \rho + V$ $\Rightarrow$ MAX FOR φ



$\nabla\varphi \parallel n$

IF I SUPPOSE ρ, g SMOOTH
(WHICH CAN BE OBTAINED BY
REGULARIZATION)

$\Rightarrow$ $T : \Omega \to \Omega$ IS A HOMEO

$T(\partial\Omega) = \partial\Omega$

$x - \nabla\varphi(x) \in \partial\Omega$

CONTRADICTION SINCE $DT \geq 0$ $\quad$ T IS MONOTONE
$\quad\quad\quad\quad\quad\quad\quad\quad\quad\quad$ $\| \quad\quad\quad\quad\quad$ $(T(x) - T(x')) \cdot (x - x') \geq 0$
$I - D^2\varphi$

$T(x)$ CANNOT BE "OPPOSITE" TO x ON $\partial\Omega$

MORE PRECISELY $\quad n(T(x)) \cdot n(x) \geq 0 \quad$ IF $\Omega = B(0,R)$ $\quad \boxed{|x - T(x)| \leq \sqrt{2}\, R}$

WHAT ABOUT $\|\nabla(\log \rho + V)\|_{L^\infty} \overset{?}{\leq}$

IF $\nabla(\log g + V) \in L^\infty \Longrightarrow \nabla(\log \rho + V) \overset{?}{\in} L^\infty$

I CAN DO SOMETHING

$$\nabla(\log \rho + V) = -\frac{\nabla \varphi}{\tau} = \frac{T(x) - x}{\tau} \Longrightarrow \|T - \mathrm{id}\|_{L^\infty} = O(\tau)$$

$\max \frac{1}{2}|\nabla\varphi|^2 > 0$ TAKE x A MAX POINT $\underline{\text{IF } x \in \mathring{\Omega}}$

$\frac{1}{2}\varphi_i\varphi_i$

$\varphi_i\varphi_{ik} = 0$ $\quad D^2\varphi\nabla\varphi = 0$

$$\boxed{\varphi_i\varphi_{ikk} + \varphi_{ik}\varphi_{ik} \leq 0}$$

AS A MATRIX IN k, k

$\varphi_i\varphi_{ikk} \leq -\varphi_{ik}\varphi_{ik} \leq 0$

$$\nabla\varphi \cdot D^3\varphi + (D^2\varphi)^2 \leq 0$$

$$\log \rho(x) = \log g(T(x)) + \log(\det(I - D^2\varphi(x)))$$

(LCE)

$$\log \rho(x) = \log g(\overset{x-\nabla\varphi(x)}{\overset{\shortparallel}{T(x)}}) + \log\left(\det\left(I - D^2\varphi(x)\right)\right)$$

SOT $A = I - D^2\varphi$

$B = A^{-1}$

$$(\log \det A)' = \mathrm{Tr}[BA']$$

SOT $\tilde\rho = \log\rho$ $\quad \tilde g = \log g$

$$\tilde\rho_i = \tilde g_h(T(x))\left(I^{hi} - \varphi_{hi}\right) + B^{hk} A^{hk}_{i}$$

$$A^{hk}_{i} = -\varphi_{ihk}$$

Times φ_i'

$$\varphi_i \tilde\rho_i = \tilde g_h(T(x))\left(\varphi_h - \underbrace{\varphi_i \varphi_{hi}}_{\geq 0}\right) - B^{hk} \underbrace{\varphi_i \varphi_{ihk}}_{\leq 0}$$

$$\geq \tilde g_h(T(x))\varphi_h$$

$$T(x) = x - \nabla\varphi(x) \neq x$$

$$\nabla\varphi \cdot \nabla\tilde\rho \geq \nabla\tilde g(T(x)) \cdot \nabla\varphi$$

$$\nabla\varphi \cdot \left(\nabla(\tilde\rho + V)\right) \geq \left(\nabla\tilde g(T(x)) + \nabla V(x)\right) \cdot \nabla\varphi$$

$$\nabla\varphi\cdot\big(\underbrace{\nabla(\hat{\rho}+V)}_{=-\frac{\nabla\varphi}{\tau}}\big) \geq \big(\nabla\tilde{g}(T(x)) + \nabla V(x)\big)\cdot\nabla\varphi \geq \big(\nabla\tilde{g}(T(x)) + \nabla V(T(x))\big)\cdot\nabla\varphi$$

SUPPOSE V IS CONVEX

$$\big(\nabla V(x) - \nabla V(T(x))\big)\cdot\big(\underbrace{x - T(x)}_{=\nabla\varphi(x)}\big) \geq 0$$

$$\frac{|\nabla\varphi|^2}{\tau} \leq -\nabla(\tilde{g}+V)(T(x))\cdot\nabla\varphi \leq |\nabla\varphi|\,\|\nabla(\tilde{g}+V)\|_{L^\infty}$$

$$\Rightarrow \frac{|\nabla\varphi|}{\tau} \leq \|\nabla(\tilde{g}+V)\|_{L^\infty}$$

$$\|\nabla(\hat{\rho}+V)\|_{L^\infty} = \left\|\frac{\nabla\varphi}{\tau}\right\|_{L^\infty}$$

IF V IS NOT CONVEX

BUT $D^2V \geq \alpha I$

$$(1+\alpha\tau)\,\|\nabla(\hat{\rho}+V)\|_{L^\infty} \leq \|\nabla(\tilde{g}+V)\|_{L^\infty}$$

WHAT ABOUT $x \in \partial\Omega$?

IF EVERYTHING IS SMOOTH

SUPPOSE $\Omega = B(0,R)$ $\qquad T(\partial\Omega) = \partial\Omega$

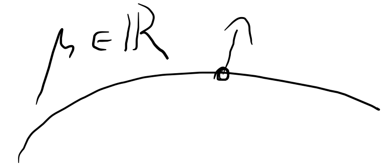
I CAN $x \notin \partial\Omega$

$$|x - \nabla\varphi(x)|^2 = R^2 \implies 2x\cdot\nabla\varphi(x) = \underline{|\nabla\varphi|^2}$$

$$\overset{\|}{|T(x)|^2} \qquad |x|^2 = R^2 \qquad \forall x \in \partial\Omega$$

$$\max_{\Omega} |\nabla\varphi|^2 \implies D^2\varphi\,\nabla\varphi = \lambda x \quad \cdot x \quad \lambda \geq 0$$

$$\max_{\partial\Omega} x\cdot\nabla\varphi \implies \nabla\varphi + x\cdot D^2\varphi = \mu x \quad \mu \in \mathbb{R}$$



$$x\cdot D^2\varphi\,\nabla\varphi = \lambda R^2 \geq 0$$

$$|\nabla\varphi|^2 + \underbrace{x\cdot D^2\varphi\cdot\nabla\varphi}_{\geq 0} = \mu\, x\cdot\nabla\varphi = \frac{\mu}{2}|\nabla\varphi|^2$$

$$\implies \mu \geq 2$$

$$\begin{cases} D^2\varphi\,\nabla\varphi = \lambda x \\ \nabla\varphi + x\cdot D^2\varphi = \mu x \end{cases} \qquad \mu \geq 0$$

$\cdot\, x$

$$\underbrace{\nabla\varphi\cdot x}_{=\frac{1}{2}|\nabla\varphi|^2} + \underbrace{x\cdot D^2\varphi\cdot x}_{<|x|^2 = R^2} = \mu|x|^2 \geq 2R^2$$

$D^2\varphi < I$

(OTHERWISE $\det = 0$)

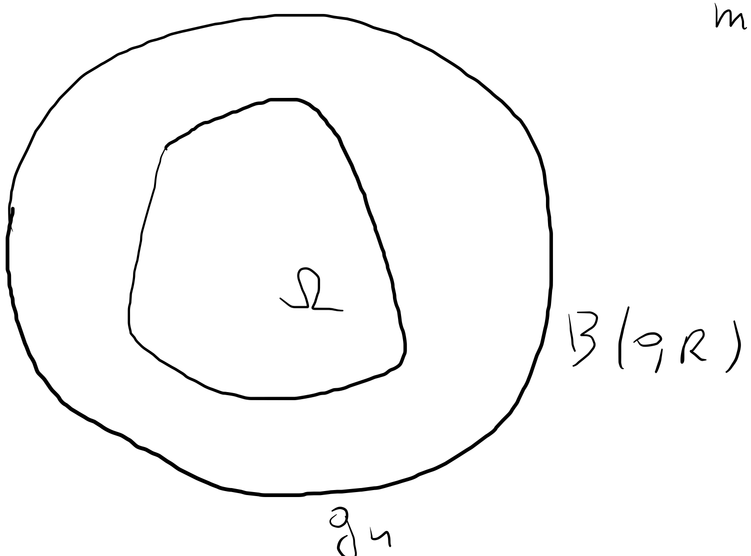
$$\Rightarrow \quad \frac{1}{2}|\nabla\varphi|^2 > R^2$$

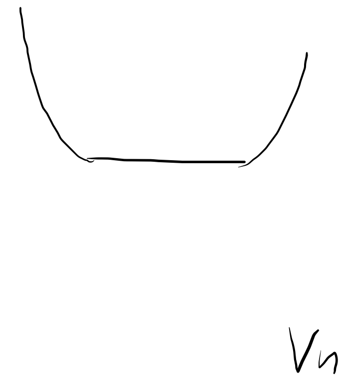
$$\underbrace{|\nabla\varphi|}_{=|x - T(x)|} > \sqrt{2}\,R$$

$\Rightarrow$ CONTRADICTION

IF Ω IS CONVEX, BDD BUT NOT A BALL

$$\min \int V_n \, d\rho + \int \rho \log \rho + \dots$$





TAKE ~~EX~~TENSIONS OF g AND EXTENSIONS OF V WITH $V_n \to +\infty$ on $B(0,R) \setminus \Omega$, $D^2 V_n \geq \alpha I$

YOU GET BOUNDS ON $\|\nabla(\tilde{\rho}_n + V_n)\|_{L^\infty(B(0,R))} \leq \dots$

$$\leq \|\nabla(\hat{\rho}_n + V)\|_{L^\infty(\Omega)}$$

$$\partial_t \rho = \nabla \cdot (\rho \vec{\cancel{v}}) + \Delta p$$

$v = \nabla V \qquad \nabla \cdot (\rho \nabla p)$

$p \geq 0 \qquad p(1-\rho) = 0$

$$\rho \in \{0, 1\}$$

$$\rho = 0 \Rightarrow \begin{cases} \Delta p = -\nabla \cdot V \\ \rho = 0 \end{cases} \qquad \partial \{\rho = 1\}$$

INNONKIN
VCVA

$$F(\rho) = \begin{cases} \int \rho V & \text{IF } \rho \leq 1 \\ +\infty & \text{IF NOT} \end{cases}$$

$\rho_0 = I_{\Omega_0}$

$\Delta V \geq 0$