$\boxed{1}$ A particle systems method to derive Wasserstein gradient flow structures

Not about connection particle ~~systems~~ and differential equations... not directly!

Indirectly (vague)

$$\begin{array}{ccc}\boxed{\text{Large Deviations}} & \text{---} & \boxed{\text{Gradient flow}} \\ | & & | \\ \boxed{\text{Brownian particles}} & \longrightarrow & \boxed{\partial_t u = u''}\end{array}$$

Gradient flow → involves ~~entropy maximisation~~

1) discuss connections
2) exploit connection to derive gradient flow structures

Gradient flow — diff. eq

(time-discrete schemes)

$\boxed{L^2}$ sequence $(\rho^j)_{j=1}^{\infty}$: Given ρ^{j-1}, let ρ^j be minimiser of :

$$\rho \mapsto \underbrace{\frac{1}{2}\int_{\mathbb{R}} |\rho'|^2\,dx}_{\substack{\text{energy}\\ E(\rho)}} + \underbrace{\frac{1}{2\tau}}_{\text{small time step}} \underbrace{\|\rho-\rho^{j-1}\|^2_{L^2(\mathbb{R})}}_{\text{metric}} \qquad (\text{in } H^1(\mathbb{R}))$$

Euler-Lagrange : $-\rho^{j\,\prime\prime} + \dfrac{\rho^j - \rho^{j-1}}{\tau} = 0$

$$\Big\downarrow \tau \to 0$$

$$\partial_t u = u'' = -\mathrm{grad}_{L^2} E(u)$$

$\boxed{\text{Wasserstein}}$

$$S(\rho) := \begin{cases} \int \rho(x)\log\rho(x)\,dx, & \rho(dx) = \rho(x)\,dx \\ \infty, & \text{otherwise} \end{cases}$$

d Wasserstein distance on $\mathcal{P}_2(\mathbb{R}^d)$

Given ρ^{j-1}, let ρ^j be minimiser of :

$$\boxed{\rho \mapsto \frac{1}{2}S(\rho) - \frac{1}{2}S(\rho^{j-1}) + \frac{1}{4\tau}d(\rho,\rho^{j-1})^2} \qquad (\mathcal{P}_2)$$

Euler Lagrange: $\text{"}\mathrm{grad}_W S(\rho^j)\text{"} + \dfrac{\rho^j - \rho^{j-1}}{\tau} = 0$

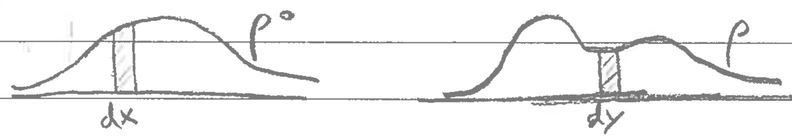
$$\Big\downarrow \tau \to 0 \qquad (*) \text{ Jordan, Kinderlehrer, Otto 1998}$$

$$\partial_t u = -\mathrm{grad}_W S(u) = u''$$

- Two competing forces.
- $\rho^{j-1} \to \rho^0$ (only interested in first transition from ρ^0 to ρ^1)

12:00

2 Wasserstein distance



$\gamma \in \mathcal{P}(\mathbb{R}\times\mathbb{R})$ transports ρ^0 to ρ if:

$$\gamma(B\times\mathbb{R}) = \rho^0(B)$$
$$\gamma(\mathbb{R}\times B) = \rho(B)$$

$\boxed{\Gamma(\rho^0,\rho) \text{ set of transport plans } \gamma \text{ from } \rho^0 \text{ to } \rho}$

$\gamma(dxdy)$ measures how much mass is transported from dx to dy

If "cost" to transport dx to dy is $|y-x|^2$, what is the minimal cost to transport ρ^0 to ρ?

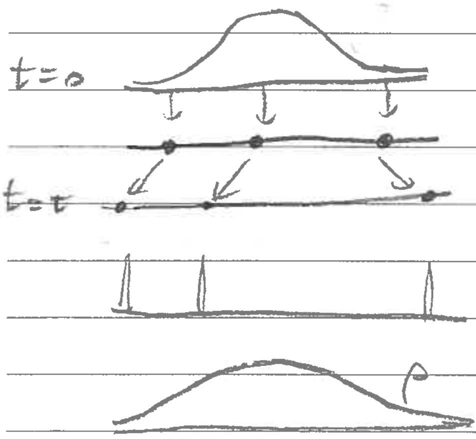
$$d(\rho^0,\rho)^2 := \inf_{\gamma\in\Gamma(\rho^0,\rho)} \iint |y-x|^2 \gamma(dxdy)$$

$$= \inf\left\{ \int_0^1 \|\partial_t \nu^t\|^2_{-1,\nu^t}\, dt : \text{curves } \nu^t \text{ s.t. } \nu^0=\rho^0 \text{ and } \nu^1 = \rho \right\}$$

$$(\nu^t \in AC((0,1):\mathcal{P}_2(\mathbb{R}))$$

15:00 $\|\partial_t \nu^t\|^2_{-1,\nu^t} = \int_{\mathbb{R}} |v^t|^2\, dx, \quad \partial_t\nu^t + \mathrm{div}(\nu^t v^t) = 0$

3 Brownian ~~Particle system~~ – diff. eq.



$\rho^0 \in \mathcal{P}_1(\mathbb{R})$ initial distribution

$X_1(0), X_2(0), \dots$ iid with law ρ^0

$\theta^t(x,y) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{(y-x)^2}{4t}\right)$ Brownian transition prob.

$$L_n(t) := \frac{1}{n}\sum_{i=1}^n \delta_{X_i(t)}$$

$L_n(t) \xrightarrow{a.s.} \mathbb{E}L_1(t) = \underbrace{\rho^0 * \theta^t}_{\text{solution of diff. eq}}$ as $n\to\infty$

$\text{Prob}(L_n(t)\in C) \to \begin{cases} 1, & \rho^0*\theta^t \in C \\ 0, & \text{otherwise} \end{cases}$ for all $C \subseteq \mathcal{P}(\mathbb{R})$ meas. ~~cont.~~ sets

→ two topologies

20:00

4 Brownian particles — Large Deviations

How fast converge to 0 or 1?

$\mathrm{Prob}(L_n(\tau)\approx\rho \mid L_n(0)\approx\rho^0) \sim \exp(-n J^\tau(\rho|\rho^0))$ as $n\to\infty$

Th Léonard 2007, Peletier-R 2011

$$J^\tau(\rho|\rho^0) = \inf_{\gamma\in\Gamma(\rho^0,\rho)} H(\gamma|\rho^0\otimes\theta^\tau) \quad \text{with} \quad H(\mu|\nu)=\begin{cases}\iint \log\left(\frac{d\mu}{d\nu}\right) d\mu, & \mu\ll\nu\\ \infty & \text{otherwise}\end{cases}$$

product measure

Th Dawson-Gärtner 1987, (Kipnis-Olla 1990)

$$J^\tau(\rho|\rho^0) = \inf\left\{\frac{1}{4}\int_0^\tau \|\partial_t\mu^s - \mu^{s''}\|^2_{-1,\mu^s}\, ds, \text{ curves with } \mu^0=\rho^0, \mu^\tau=\rho\right\}$$

5 Large Deviations — Gradient flows

→ only has to work for small τ.

Th Adams, Dirr, Peletier, Zimmer 2010; Duong, Laschos, R. 2012

$$J^\tau(\rho|\rho^0) \approx \frac{1}{2}S(\rho) - \frac{1}{2}S(\rho^0) + \frac{1}{4\tau}d(\rho^0,\rho)^2 \quad \text{as} \quad \tau\to 0$$

(Development in terms of Γ-convergence)

~~summary~~

conclusion: entropy-WS minimisation = likelihood maximization

30:00

6 New gradient flow structures

How to find GF-structure for different PDE?

1. Describe particle system by transition prob.
2. Calculate conditional LDP $J^\tau(\rho|\rho^0)$
3. Asymptotic developments of J^τ for small τ
4. Prove GF-structure

(A) Fokker–Planck

$$\partial_t u = u'' + \operatorname{div}(u \Psi') \quad \text{for some potential } \Psi$$

- transition prob: fundamental solution
- Asympt. development LDP:

Th (Peletier–R 2011, Duong, Laschos–R 2012)

$$\boxed{J^t(\rho|\rho^0) \approx \tfrac{1}{2}S(\rho) + \tfrac{1}{2}\int \Psi d\rho - \tfrac{1}{2}S(\rho^0) - \tfrac{1}{2}\int \Psi d\rho^0 + \tfrac{1}{4t} d(\rho;\rho)^2}$$

- prove GF structure:
  (Jordan, Kinderlehrer, Otto 1998)

(B) Diffusion with bulk decay

$$\partial_t u = u'' - \lambda u, \quad \text{for some } \lambda > 0$$

Not mass-conserving $\Rightarrow$ add 'decayed matter' and assume it continues its Brownian motion. State space $= \mathbb{R} \times \{N, D\}$

normal ↑ (N) ↑ dark (D)

- transition prob: indep. { Brownian motion $- \theta^t$; Decay: $\text{Prob}(N \to N) = e^{-\lambda\tau}$
  $\text{Prob}(N \to D) = 1 - e^{-\lambda\tau}$
  $\text{Prob}(D \to N) = 0$
  $\text{Prob}(D \to D) = 1$

- Asympt. development LDP. Only works if you know

Th Peletier–R 2011

$$J^t(\rho_N, \rho_{ND}, \rho_{DD} | \rho_N^0, \rho_D^0) \approx \tfrac{1}{2}S(\rho_N + \rho_{ND}) - \tfrac{1}{2}S(\rho_N^0) + \tfrac{1}{4\tau} d(\rho_N^0, \rho_N + \rho_{ND})^2$$
$$+ \tfrac{1}{2}S(\rho_{DD}) - \tfrac{1}{2}S(\rho_D^0) + \tfrac{1}{4\tau} d(\rho_D^0, \rho_{DD})^2$$
$$- S(\rho_N + \rho_{ND}) + S(\rho_N) + S(\rho_{ND}) - \|\rho_N\| \log(e^{-\lambda\tau}) - \|\rho_{ND}\| \log(1 - e^{-\lambda\tau})$$

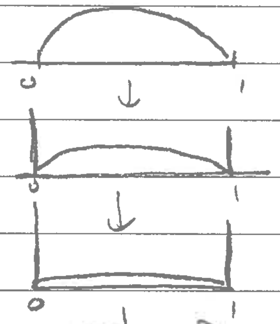
drive diffusion

drives decay; minimal if $\rho_N = e^{-\lambda\tau}(\rho_N + \rho_{ND})$

(c) Diffusion with decay at boundary

$$\begin{cases} \partial_t u = u'' & \text{in } (0,1) \\ u(0) = u(1) = 0 \end{cases}$$

Not mass-conserving → add 'decayed' mass at boundary:



- transition prob: Brownian motion with "sticking boundary"
- work in progress... it seems that

$$J^{\tau}(\rho \mid \rho^0) \approx \inf_{\substack{\rho^0_{u\ell}+\rho^0_{uin}+\rho^0_{ur} \\ \|\rho^0_{uin}\| = \|\rho\|}} \left\{ \tfrac{1}{2} S(\rho) - \tfrac{1}{2} S(\rho^0_{uin}) + S(\rho^0_{u\ell}) + S(\rho^0_{uin}) + S(\rho^0_{ur}) - S(\rho^0) \right\}$$

$$- \inf \left\{ \int_0^1\!\!\int_0^1 |y-x|^2 \gamma(dx\,dy) : \gamma \in \mathcal{P}([0,1]\times[0,1]) : \begin{array}{l} \gamma(B \times [0,1]) = \rho^0(B) \\ \gamma([0,1] \times B) = \rho(B),\ B \subset (0, \\ \gamma(\{0,1\} \times (0,1)) = 0 \end{array} \right\}$$

- similar to metric proposed in Figalli-Gigli 2011.
- only this one is assymetric!

<u>Conclusion</u>

- This method can provide new Wasserstein gradient flow structures.
- Thus found gradient flows are meaningful as a measure for unlikeliness.