Gradient flows, interpolations and large deviations

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co-authors

- Ivan Gentil
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+ thanks to Giovanni Conforti for stimulating conversations

aim

build interpolations related to the dissipation mechanism of a gradient flow

1. gradient flows in $\mathrm{P}(\mathbb{R}^n)$
2. interpolations in $\mathbb{R}^n$
3. interpolations in $\mathrm{P}(\mathbb{R}^n)$

interpolations

quadratic optimal transport

$$W_2^2(\alpha,\beta) := \inf_{\pi:\pi_0=\alpha,\pi_1=\beta} \int_{\mathbb{R}^n\times\mathbb{R}^n} |y-x|^2\,\pi(dxdy), \qquad \alpha,\beta \in \mathrm{P}(\mathbb{R}^n)$$

- $0 \le s \le 1, \qquad \Omega = C([0,1],\mathbb{R}^n)$
- $\mu \in C([0,1],\mathrm{P}(\mathbb{R}^n))$
- $\mathcal{A}(\mu) := \inf\left\{E_P \int_{[0,1]} |\dot{X}_s|^2/2\; ds;\; P \in \mathrm{P}(\Omega) : P_s = \mu_s,\ \forall 0 \le s \le 1\right\}$

displacement interpolation between α and β

$$\inf\{\mathcal{A}(\mu) : \mu : \mu_0 = \alpha, \mu_1 = \beta\} = W_2^2(\alpha,\beta)$$

interpolations

- displacement interpolations are the constant speed geodesics (in a metric sense) of the *Wasserstein geometry* on $\mathrm{P}(\mathbb{R}^n)$, [Otto]

Benamou-Brenier formula

$$W_2^2(\alpha,\beta) = \inf_{(\nu,v)} \int_{[0,1]\times\mathbb{R}^n} |v_s|^2 \; d\nu_s ds = \inf_{\nu} \int_{[0,1]} \|\dot\nu_s\|^2_{\nu_s} \; ds$$

- $\partial_s \nu + \mathrm{div}(\nu v) = 0$

- $\|\dot\nu_s\|^2_{\nu_s} := \inf_{v : \partial_s \nu + \mathrm{div}(\nu v) = 0} \int_{\mathbb{R}^n} |v|^2 \, d\nu_s$

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    - $\partial_s \nu + \mathrm{div}(\nu\dot{\nu}) = 0$
    - $\dot{\nu} = \nabla\phi$

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- displacement interpolations are not regular
- ϵ-*entropic interpolations* are regular approximations

gradient flows

Fokker-Planck equation

$$\partial_t m - \operatorname{div}(mU'/2) = \Delta m/2$$

- $m_t \in \mathrm{P}(\mathbb{R}^n), \qquad t \geq 0$
- $U : \mathbb{R}^n \to \mathbb{R}$

gradient flows

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- $U : \mathbb{R}^n \to \mathbb{R}$

- hypothesis: $\qquad U'' \geq \kappa \mathrm{Id}, \quad \kappa > 0$
  - $m_t = \mathcal{S}_t(m_0), \qquad$ semi-group
  - $m_\infty := \lim_{t\to\infty} m_t = e^{-U}\,\mathrm{Leb}$

gradient flows

JKO

$t \mapsto m_t$ is the W_2-gradient flow in $\mathrm{P}(\mathbb{R}^n)$ of $\mathcal{F} := \frac{1}{2} H(\cdot|m_\infty)$

- free energy: $\mathcal{F}(\alpha) = \frac{1}{2}[\int_{\mathbb{R}^n} U\, d\alpha + H(\alpha|\mathrm{Leb})], \quad \alpha \in \mathrm{P}(\mathbb{R}^n)$
  - relative entropy: $H(\alpha|m) := \int_{\mathbb{R}^n} \log(d\alpha/dm)\, d\alpha$
- $\dot{\mu}_t = -\,\mathrm{grad}^W_{\mu_t} \mathcal{F}$

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1. $(m_t)_{t\geq 0}$ is also the gradient flow of $\mathcal{F}$ with respect to a *large deviation cost*
2. this large deviation cost leads to the *regular* ϵ-entropic interpolations

gradient flows

- state space: $\mathcal{X} = \mathbb{R}^n$
  - warming up serving as an analogy, before $\mathcal{X} = \mathrm{P}(\mathbb{R}^n)$
- path: $\omega = (\omega_t)_{t \geq 0} \in C([0,\infty), \mathbb{R}^n) =: \Omega_\infty$
- free energy: $F : \mathbb{R}^n \to \mathbb{R}$

$$\dot{\omega}_t = -F'(\omega_t), \quad t \geq 0$$

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results

hypothesis: $F'' \geq K\mathrm{Id}, \quad K > 0$

- semigroup: $\omega_t = \mathsf{S}_t(\omega_0), \quad t \geq 0$
- contraction: $|\mathsf{S}_t(x) - \mathsf{S}_t(y)| \leq e^{-Kt}[x - y], \quad t \geq 0$
  $|\mathsf{S}_t(x) - x_*| \leq e^{-Kt}|x - x_*|$
  - $x_* = \operatorname{argmin} F$: equilibrium state

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- free energy dissipation: $\dfrac{d}{dt}F(\omega_t) = F'(\omega_t)\cdot\dot{\omega}_t = -|F'|^2(\omega_t) \leq 0$
  - $I = |F'|^2 : \mathcal{X} \to [0,\infty)$

gradient flows

slowing down: $\epsilon \to 0^+$

- $\omega_t^\epsilon := \omega_{\epsilon t}, \qquad \dot{\omega}_t^\epsilon = \epsilon \dot{\omega}_{\epsilon t} = -\epsilon F'(\omega_t^\epsilon), \qquad F \rightsquigarrow \epsilon F$

gradient flows

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- $\ddot\omega_t^\epsilon = -\epsilon \frac{d}{dt} F'(\omega_t^\epsilon) = \epsilon^2 F'' F'(\omega_t^\epsilon) = \epsilon^2 \left(|F'|^2/2\right)' (\omega_t^\epsilon)$

Newton's equation

$$\ddot\omega_t^\epsilon = -\epsilon^2 V'(\omega_t^\epsilon), \qquad V = -I/2 = -|F'|^2/2$$

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along the gradient flow, the force field is the gradient of (half) the free energy dissipation

- $\dfrac{d}{dt} F(\omega_t^\epsilon) = -|\epsilon F'|^2(\omega_t^\epsilon)$

interpolations

building interpolations related to this free energy dissipation force field

1. $\begin{cases} \dot{\omega} &= -F'(\omega) \\ \omega_0 &= x^0 \end{cases}$ iff it solves $\displaystyle \inf_{\omega:\omega_0=x^0} \int_{[0,\infty)} \frac{1}{2} |\dot{\omega}_t + F'(\omega_t)|^2 \, dt$
   - this serves as a definition (minimizing movement)

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   - this serves as a definition (minimizing movement)
2. small time step: $\epsilon > 0$, $\Omega^{xy} := \{\omega \in \Omega;\ \omega_0 = x, \omega_1 = y\}$

$$\inf_{\omega:\omega_0=x,\omega_\epsilon=y} \int_{[0,\epsilon]} \frac{1}{2}|\dot\omega_t + F'(\omega_t)|^2\, dt$$

$$= F(y) - F(x) + \epsilon^{-1} \inf_{\omega\in\Omega^{xy}} \int_{[0,1]} \left\{ \frac{|\dot\omega_s|^2}{2} + \epsilon^2 \frac{|F'|^2(\omega_s)}{2} \right\} ds$$

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3. $A^\epsilon(\omega):=\int_{[0,1]}L^\epsilon(\omega_s,\dot\omega_s)\,ds=\int_{[0,1]}\left\{\frac{|\dot\omega_s|^2}{2}+\epsilon^2\frac{I(\omega_s)}{2}\right\}\,ds$
4. $\inf_{\omega\in\Omega^{xy}}A^\epsilon(\omega)=:C_{\epsilon F}(x,y)$

interpolations

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ϵF-cost, ϵF-interpolation

$$\inf_{\omega \in \Omega^{xy}} A^\epsilon(\omega) =: C_{\epsilon F}(x, y)$$

- $C_{\epsilon F}(x, y) = |y - x|^2/2 + O(\epsilon^2)$,
- $\gamma^{\epsilon, xy} \underset{\epsilon \to 0^+}{\to} \gamma^{xy}$

interpolations

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interpolations and dissipation

along the ϵF-interpolations, the force field is (half) the gradient of the free energy dissipation of the ϵ-slowed down gradient flow

interpolations

ϵ-modified contraction of the gradient flow in $\mathbb{R}^n$

$$C_{\epsilon F}(\mathsf{S}_t(x), \mathsf{S}_t(y)) \leq e^{-2Kt} C_{\epsilon F}(x, y), \quad \forall t, x, y$$

- $|\mathsf{S}_t(x) - \mathsf{S}_t(y)|^2 \leq e^{-2Kt}|x - y|^2$

interpolations

"ϵ-modified K-convexity" of F

for any ϵF-*interpolation* γ and all $0 \le s \le 1$

$$F(\gamma_s) \le \theta_{\epsilon K}(1-s)F(\gamma_0) + \theta_{\epsilon K}(s)F(\gamma_1) \\ - \frac{1-e^{-2\epsilon K}}{2\epsilon}\theta_{\epsilon K}(s)\theta_{\epsilon K}(1-s)\big[C_{\epsilon F}(\gamma_0,\gamma_1) + \epsilon F(\gamma_0) + \epsilon F(\gamma_1)\big]$$

- $\theta_{\epsilon K}(s) := \dfrac{1-e^{-2\epsilon K t}}{1-e^{-2\epsilon K}} \underset{\epsilon \to 0^+}{\longrightarrow} s$
- K-convexity of F: for any *geodesic* γ and all $0 \le s \le 1$

$$F(\gamma_s) \le (1-s)F(\gamma_0) + sF(\gamma_1) - Ks(1-s)|\gamma_1 - \gamma_0|^2/2$$

interpolations

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- thank you Giovanni

interpolations

ϵ-modified basic convexity inequality

$$C_{\epsilon F}(y, x_*) \le \frac{\epsilon}{\tanh(K\epsilon)} \, [F(y) - F(x_*)], \quad \forall y$$

- $s = 0, \ \gamma_0 = x_*$
- $\epsilon \to 0^+$ leads to $\quad [F(y) - F(x_*)] \ge K|y - x_*|^2/2, \ \forall y$

large deviations

- Fokker-Planck equation: $\partial_t m - \mathrm{div}(mU'/2) = \Delta m/2$

- $(m_t)_{t\geq 0}$ a gradient flow with respect to a *large deviation cost*
- this large deviation cost gives *regular* interpolations

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- stochastic representation of (m_t)
  - $\begin{cases} dZ_t = -U'(Z_t)/2\ dt + dW_t, & t \geq 0 \\ Z_0 \sim m_0 \end{cases}$
  - Markov generator: $(-U' \cdot \nabla + \Delta)/2$
  - $R^{m_0} = \mathrm{Law}(Z) \in \mathrm{P}(\Omega_\infty)$
  - $m_t = \mathrm{Law}(Z_t) = R_t^{m_0} \in \mathrm{P}(\mathbb{R}^n)$

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  - $m_t = \mathrm{Law}(Z_t) = R_t^{m_0} \in \mathrm{P}(\mathbb{R}^n)$
- $R := R^{m_\infty}$ is m_∞-reversible

large deviations

- particle system: $Z^1, Z^2, \dots$ iid(R)
- empirical measures: $\widehat{Z}^N := N^{-1} \sum_{1\le i\le N} \delta_{Z^i} \in \mathrm{P}(\Omega_\infty)$

$$\overline{Z}^N := (\widehat{Z}^N_t)_{t\ge 0} \in \mathcal{C} := C([0,\infty), \mathrm{P}(\mathbb{R}^n))$$

$$\widehat{Z}^N_t = \overline{Z}^N_t \in \mathrm{P}(\mathbb{R}^n), \quad t \ge 0$$

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- large deviations as $N \to \infty$

(by Sanov's theorem)

$$\mathbb{P}(\widehat{Z}^N \in \cdot) \underset{N\to\infty}{\asymp} \exp\Big(- N \inf_{P\in\cdot} H(P|R)\Big)$$

- $H(P|R) := \int_\Omega \log(dP/dR)\, dP, \qquad P \in \mathrm{P}(\Omega_\infty)$

large deviations

(by the contraction principle)

$$\mathbb{P}(\overline{Z}^N \simeq \mu \mid \overline{Z}_0^N \simeq m_0) \underset{N\to\infty}{\asymp} \exp\left(-NJ_{m_0}(\mu)\right), \qquad \mu \in \mathcal{C}$$

- $J_{m_0}(\mu) = \inf\left\{H(P|R^{m_0});\ P : P_t = \mu_t,\ \forall t \geq 0\right\} + \iota_{\{\mu_0 = m_0\}}$

large deviations

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- argmin $J_{m_0} = (m_t)_{t\geq 0}$
- strong LLN: knowing that $\lim_{N\to\infty} \overline{Z}_0^N = m_0$, *as*, we have:

$$\lim_{N\to\infty} \overline{Z}^N = (m_t)_{t\geq 0}$$

- $P = R^{m_0} \implies P_t = R_t^{m_0} = m_t$

interpolations

building interpolations related to this free energy dissipation force field

- $$\int_{[0,\epsilon]} \frac{1}{2}|\dot{\omega}_t + F'(\omega_t)|^2\, dt$$
$$= F(\omega_\epsilon) - F(\omega_0) + \epsilon^{-1} \int_{[0,1]} \left\{ \frac{|\dot{\omega}_s|^2}{2} + \epsilon^2 \frac{|F'|^2(\omega_s)}{2} \right\} ds$$

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- $J_{m_0}(\mu) = \inf\{H(P|R^{m_0});\ P : P_t = \mu_t,\ \forall t \geq 0\} + \iota_{\{\mu_0 = m_0\}}$
- $\mathcal{F}(\alpha) = \frac{1}{2} H(\alpha|m_\infty)$
- $\mathcal{A}^\epsilon(\mu) := \epsilon \inf\left\{\frac{1}{2}[H(P|R^{\epsilon,\alpha}) + H(P^*|R^{\epsilon,\beta})]; P : P_s = \mu_s, 0 \leq s \leq 1\right\}$
  - small time interval: $[0,\epsilon]$
  - slowing down: $[0,\epsilon] \to [0,1]$, $R^\epsilon := (X_{\epsilon \bullet})_\# R$
  - time reversal: $P^* := (X^*)_\# P$, $X^*_s := X_{1-s}$, $0 \leq s \leq 1$
    $R^* = R$

interpolations

ϵ-entropic interpolation

$$\inf\{\mathcal{A}^\epsilon(\mu);\ \mu : \mu_0 = \alpha, \mu_1 = \beta\} =: C^\epsilon_{LD}(\alpha, \beta), \quad \alpha, \beta \in \mathrm{P}(\mathbb{R}^n)$$

- Schrödinger problem (1931)

- C^ϵ_{LD} : large deviation cost

interpolations

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- Schrödinger problem (1931)

- C^ϵ_{LD} : large deviation cost
- by the way . . . where is the free energy dissipation?

interpolations

- $W_2^2(\alpha,\beta) = \inf_{(\nu,v)} \int_{[0,1]\times\mathbb{R}^n} |v_s|^2 \; d\nu_s ds = \inf_{\nu} \int_{[0,1]} \|\dot\nu_s\|^2_{\nu_s} \; ds$

ϵ-modified Benamou-Brenier formula (ref. [CGP], [GLR])

$$C^{\epsilon}_{LD}(\alpha,\beta) = \inf_{\nu} \int_{[0,1]} \left\{ \frac{\|\dot\nu_s\|^2_{\nu_s}}{2} + \epsilon^2 \frac{\mathcal{I}(\nu_s|m_\infty)}{2} \right\} ds$$

- $\mathcal{I}(\alpha|m_\infty) := \int_{\mathbb{R}^n} |\nabla \log \sqrt{d\alpha/dm_\infty}|^2 \; d\alpha$ (Fisher information)
  - time reversal
  - Nelson's stochastic velocities
- depends on α, not on velocity
- *regularizing effect*

interpolations

- $C^{\epsilon}_{LD}(\alpha,\beta) = \inf_{\nu} \int_{[0,1]} \left\{ \frac{\|\dot{\nu}_s\|^2_{\nu_s}}{2} + \epsilon^2 \frac{\mathcal{I}(\nu_s|m_\infty)}{2} \right\} ds$
  - compare: $C_{\epsilon F}(x,y) := \inf_{\omega\in\Omega^{xy}} \int_{[0,1]} \left\{ \frac{|\dot{\omega}_s|^2}{2} + \epsilon^2 \frac{|F'|^2(\omega_s)}{2} \right\} ds$
    $I = |F'|^2$

results

- $\mathcal{I}(\alpha|m_\infty) = \|\operatorname{grad}^W_\alpha \mathcal{F}\|^2_\alpha$
- $\Gamma\text{-}\lim_{\epsilon\to 0^+}(C^{\epsilon}_{LD}) = (W_2^2/2)$

interpolations

- $U'' \geq \kappa \mathrm{Id}$
- $K := \kappa/2$

ϵ-modified contraction of the gradient flow in $\mathrm{P}(\mathbb{R}^n)$

$$C^{\epsilon}_{LD}(\mathcal{S}_t(\alpha), \mathcal{S}_t(\beta)) \leq e^{-2Kt} C^{\epsilon}_{LD}(\alpha, \beta), \quad \forall t \geq 0, \ \forall \alpha, \beta \in \mathrm{P}(\mathbb{R}^n)$$

- $W_2^2(\mathcal{S}_t(\alpha), \mathcal{S}_t(\beta)) \leq e^{-2Kt} W_2^2(\alpha, \beta)$

interpolations

"ϵ-modified K-convexity" of $\mathcal{F}$ (Conforti)

for any *entropic ϵ-interpolation* μ and all $0 \le s \le 1$

$$\mathcal{F}(\mu_s) \le \theta_{\epsilon K}(1-s)\mathcal{F}(\mu_0) + \theta_{\epsilon K}(s)\mathcal{F}(\mu_1) - \frac{1-e^{-2\epsilon K}}{2\epsilon}\theta_{\epsilon K}(s)\theta_{\epsilon K}(1-s)\left[C^{\epsilon}_{LD}(\mu_0,\mu_1) + \epsilon\mathcal{F}(\mu_0) + \epsilon\mathcal{F}(\mu_1)\right]$$

- for any displacement interpolation μ and all $0 \le s \le 1$

  $$\mathcal{F}(\mu_s) \le (1-s)\mathcal{F}(\mu_0) + s\mathcal{F}(\mu_1) - Ks(1-s)W_2^2(\mu_0,\mu_1)/2$$

interpolations

ϵ-modified Talagrand inequality

$$C_{LD}^{\epsilon}(\alpha, m_\infty) \le \frac{\epsilon}{\tanh(K\epsilon)}\,\mathcal{F}(\alpha), \quad \forall \alpha \in \mathrm{P}(\mathbb{R}^n)$$

- $$W_2^2(\alpha, m_\infty)/2 \le K^{-1}\mathcal{F}(\alpha), \quad \forall \alpha$$

gradient flows, interpolations and large deviations

1. LD of empirical mesures of diffusive particles
2. LD rate function: $J(\mu)$ & slowing down: $[0, \epsilon]$

$$\downarrow$$

free energy: $\mathcal{F}(\alpha)$ & LD cost: $C^{\epsilon}_{LD}(\alpha, \beta)$

3. identify the free energy dissipation: $\mathcal{I}(\alpha)$

gradient flows, interpolations and large deviations

$\epsilon\mathcal{F}$-interpolations are well-suited approximations of displacement interpolations:

- they allow for proving tight perturbations of transport inequalities involving $\mathcal{F}$
- they inherit some regularity from the dissipative mechanism (if any) of the gradient flow

gradient flows, interpolations and large deviations

$\epsilon\mathcal{F}$-interpolations are well-suited approximations of displacement interpolations:

- they allow for proving tight perturbations of transport inequalities involving $\mathcal{F}$
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- rigorous proofs in the present setting
- extension to other free energy functions $\mathcal{F}$, undone at present time, but the heuristics are known
  - Conforti: arXiv:1704.04821 (PTRF online)
  - Gentil-L-Ripani: arXiv:1806.01553

thank you for your attention