Motivation (Jordan–Kinderlehrer–Otto '98). J. Maas 19/01/2014.

Connection b/w:

- 2-Wasserstein metric:

$$W_2(\mu,\nu) = \inf_{\gamma} \left\{ \iint_{\mathbb{R}^n\times\mathbb{R}^n} |x-y|^2 \, d\gamma(x,y) : \begin{array}{l} \gamma(A\times\mathbb{R}^n) = \mu(A) \\ \gamma(\mathbb{R}^n\times B) = \nu(B) \end{array} \right\}.$$

- Boltzmann entropy for $\mu \in \mathcal{P}(\mathbb{R}^n)$.

$$H(\mu) = \begin{cases} \int \rho(x) \log\rho(x)\, dx & d\mu = \rho(x)\,dx \\ +\infty & \text{otherwise}. \end{cases}$$

Th^m The heat equation $\partial_t \rho = \Delta\rho$ in $\mathbb{R}^n$ is the gradient flow of H w.r.t. to W_2.

One interpretation: fix $\mu \in \mathcal{P}(\mathbb{R}^n)$, define

$$J_h \mu = \operatorname*{argmin}_{\nu} \left\{ H(\nu) + \frac{1}{2h} W_2^2(\mu,\nu) \right\}.$$

Then, $\mu_t := \lim_{n\to\infty} \left(J_{t/n}\right)^n \mu$ exists and satisfies

$$\partial_t \mu_t = \Delta \mu_t, \quad \mu|_{t=0} = \mu.$$

Point: Holds in very general metric ~~spaces~~ measure spaces. (Ambrosio–Gigli–Savaré).

What about discrete spaces?

<u>Example</u>: $\mathcal{X} = \{0,1\}$, $\mathcal{P}(\mathcal{X}) = \{\mu_\alpha = (1-\alpha)\delta_0 + \alpha\delta_1 : \alpha \in [0,1]\}$.

Then. $W_2(\mu_\alpha, \mu_\beta) = \sqrt{|\alpha - \beta|}$. Thus, $(\mathcal{P}(\mathcal{X}), W_2) \cong ([0,1], \sqrt{|\cdot - \cdot|})$

Very <u>bad</u> metric space.

Now, let $f : [0,1] \to \mathbb{R}$ smooth, endow $[0,1]$ with.
$d(x,y) = \sqrt{|x-y|}$, Then, try minimisation scheme:

$\forall x \in [0,1]$. $\qquad \arg\min_y \{ f(y) + \frac{1}{2h} |x-y| \} = x$.

if $h > 0$ is small.

Ie, all gradient flows are just <u>constant</u>!.

<u>Discrete Setting</u>

- $\mathcal{X}$ finite set.
- $\mathcal{L}$ generator of continuous-time Markov chain.

$$\mathcal{L}\psi(x) = \sum_y Q(x,y)(\psi(y) - \psi(x)).$$

discrete analogue of Laplacian.

$$Q(x,y) \geq 0, \quad Q(x,x) = 0.$$

- $\exists$ prob measure π on $\mathcal{X}$ s.t. $\forall x, y$.

$$\pi(x) Q(x,y) = \pi(y) Q(y,x). \quad \text{(detailed balance eq}^{\text{n}}\text{s)}.$$

- Heat semigroup $(e^{t\mathcal{L}})_{t \geq 0}$ is self-adjoint on $L^2(\mathcal{X}, \pi)$.

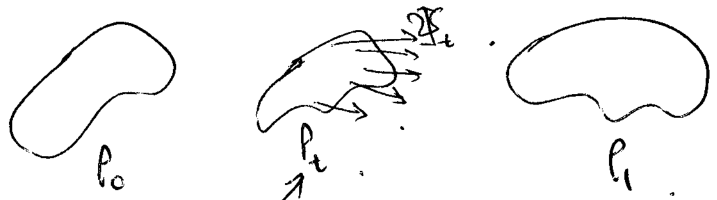
• Dirichlet energy $\mathcal{E} : L^2(\mathcal{X},\pi) \to \mathbb{R}$.

• $$\mathcal{E}(\psi) = \frac{1}{2} \sum_{x,y} (\psi(x) - \psi(y))^2 \, w(x,y).$$

<u>Exercise</u>: the heat equation $\partial_t \psi = \mathcal{L}\psi$ is the gradient flow of $\mathcal{E}$ w.r.t $L^2(\mathcal{X},\pi)$.

<u>Back to $\mathbb{R}^n$</u>: for $\rho_0(dx) = \rho_0(x)\,dx$, $\rho_1(dx) = \rho_1(x)\,dx$.

Benamou-Brenier formula:



follow entire trajectories.

but consider as a cloud of particles.

$\rightsquigarrow$ get velocity vectors Φ_t

Then,
$$W_2(\rho_0,\rho_1)^2 = \inf_{\rho,\Phi_t} \left\{ \int_0^1 \int_{\mathbb{R}^n} |\Phi_t|^2 \, d\rho_t(x)\, dt : \begin{array}{l} \partial_t \rho + \mathrm{div}(\rho\Phi) = 0 \\ \rho|_{t=0} = \rho_0, \ \rho|_{t=1} = \rho_1 \end{array} \right\}.$$

Use this as motivation for discrete case.

$\boxed{\text{N.b. } \cancel{\text{At}} \text{ each } t, \ \exists \psi \text{ s.t. } \Phi_t = \nabla \psi_t.}$

Notation: • $E = \{(x,y) \in \mathcal{X}\times\mathcal{X} : Q(x,y) > 0\}$.

• for functions $\psi : \mathcal{X} \to \mathbb{R}$, set
$$\nabla\psi(x,y) = \psi(y) - \psi(x).$$

| Gradient is vector, so defined on ~~edges~~ edges (x,y) |

• for vector fields $\Phi : E \to \mathbb{R}$, set
$$(\mathrm{div}\,\psi)(x) = \frac{1}{2} \sum_y (\Phi(x,y) - \Phi(y,x))\, Q(x,y).$$

Also, $\langle \nabla \psi, \Psi \rangle_{L^2(E,w)} = \langle \psi, \operatorname{div} \Psi \rangle_{L^2(X,\pi)}$.

and $L_K \psi = \operatorname{div} \nabla \psi$.

<u>Need:</u> ~~A~~ to multiply functions and vectorfields?

~~Ex~~

Fix $\theta : \mathbb{R}_+ \times \mathbb{R}_+ \to \mathbb{R}_+$ smooth, symmetric, and $\theta(s,t) > 0$ for $s,t > 0$.

For $\rho : X \to \mathbb{R}_+$, set $\hat{\rho}(x,y) = \theta(\rho(x), \rho(y))$.

$\mathcal{P}(X) = \{ \rho : X \to \mathbb{R}_+ : \sum \rho(x)\pi(x) = 1 \}$.

<u>Prop</u> Let $\rho \in \mathcal{P}_{>0}(X) = \{ \rho \in \mathcal{P}(X) : \rho > 0 \}$, and $(\rho_t)_{t \in (-\varepsilon,\varepsilon)}$ be smooth with $\rho_0 = \rho$. Then $\exists ! \Psi : E \to \mathbb{R}$ s.t.

- $\Psi = \nabla \psi$ for some $\psi : X \to \mathbb{R}$.
- $\dot{\rho}_0 + \nabla \cdot (\hat{\rho} \Psi) = 0$. (Continuity eq^{n})

<u>Note:</u> This depends on choice of θ.

<u>A Riemannian structure:</u>

(I) for any probability density $\rho > 0$, identify tangent space at ρ with $\{ \nabla \psi : \psi : X \to \mathbb{R} \}$ using identification given by continuity equation.

(II). For $\rho \in \mathcal{P}_{>0}(X)$, define $\langle \nabla \psi, \nabla \varphi \rangle_\rho := \langle \hat{\rho} \nabla \psi, \nabla \varphi \rangle_{L^2(X,\mu)}$.

<u>Note:</u> The Riemannian distance is given by

$$W(\rho_0, \rho_1)^2 = \inf \left\{ \int_0^1 \langle \hat{\rho}_t \nabla \psi_t, \nabla \psi_t \rangle_{L^2(E,\mu)} \, dt \ \text{ s.t. } \partial_t \rho + \nabla \cdot (\hat{\rho} \nabla \psi_t) = 0 \right\}$$

Note: Typically, ~~differentiate~~ Tangent space. at $\rho \in \mathcal{P}_o(\mathcal{X})$, ~~we~~

We find curve ρ_t and write. a vector.

$$\partial_t|_{t=0} \rho_t .$$

But continuity eq^n:

$$\partial_t \rho_t + \nabla \cdot (\hat{\rho}_t \nabla \psi_t) = 0.$$

means that we can identify such curves with $\{\nabla \psi_t\}$.

Note: $\mathcal{W}(\rho_0, \rho_1)$ is not Wasserstein metric in discrete setting.

Def^n: $\mathcal{H}(\rho) = \sum_y \rho(y) \log \rho(y)\, dy$.

Th^m. The heat eq. $\partial_t \rho = \Delta \rho$ is the ~~heat~~ gradient flow equation of $\mathcal{H}$ w.r.t. $\mathcal{W}$, provided that.

$$\theta(s,t) =: \int_0^1 s^{1-\alpha} t^{\alpha}\, d\alpha = \frac{s-t}{\log(s) - \log(t)}.$$

Pf. Let (ρ_t) satisfy $\partial_t \rho_t + \nabla \cdot (\hat{\rho}_t \nabla \psi) = 0$. Then,

$$\partial_t \mathcal{H}(\rho_t) = \langle 1 + \log \rho_t, \partial_t \rho_t \rangle_\pi = \langle 1 + \log \rho_t + \nabla \cdot (\hat{\rho}_t \nabla \psi_t) \rangle$$

$$= \langle \nabla \log \rho_t, \hat{\rho} \nabla \psi_t \rangle_{\mathcal{W}}.$$

$$\Rightarrow \operatorname{grad}_{\mathcal{W}} \mathcal{H}(\rho_t) = \nabla \log \rho_t .$$

Thus, the gradient flow of $\mathcal{H}$ is given by

$$\partial_t \rho_t - \nabla \cdot (\hat{\rho}_t \nabla \log \rho_t) = 0 .$$

Now; $\hat{\rho}(x,y)\,\nabla \log \rho(x,y) = \theta(\rho(x),\rho(y))\,(\log \rho(x) - \log \rho(y)) = \rho(x) - \rho(y).$ $\boxed{4}$

<u>Exercise</u> Show that the discrete porous medium equation.

$$\partial_t \rho = \Delta \varphi(\rho) \quad , \quad \varphi : \mathbb{R} \to \mathbb{R} \text{ increasing}.$$

is the gradient flow of the functional.

$$\mathcal{F}(\rho) = \sum_x f(\rho(x))\,\pi(x). \qquad \text{w.r.t. } \mathcal{W}.$$

if $$\theta(s,t) = \frac{\varphi(s) - \varphi(t)}{f'(s) - f'(t)}.$$