Gradient Flows and Optimal Transport in Discrete and Quantum Systems

Jan Maas (IST Austria)

Geometric Methods in Optimization and Sampling Boot Camp

Simons Institute

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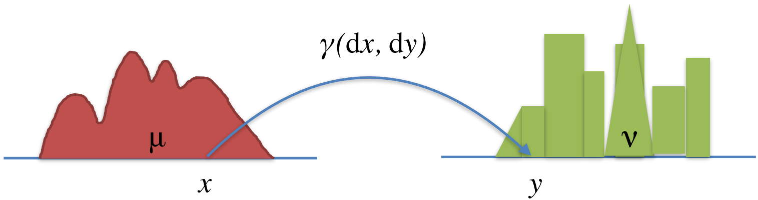
IST AUSTRIA

Institute of Science and Technology

Starting point:

Diffusion equations and Ricci curvature
via optimal transport

Optimal transport



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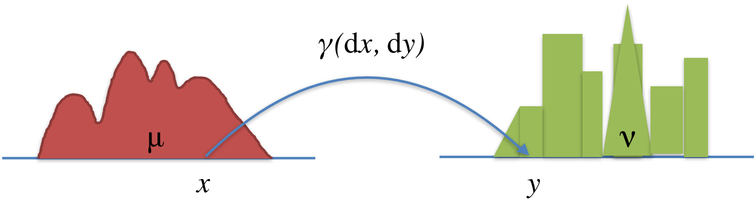

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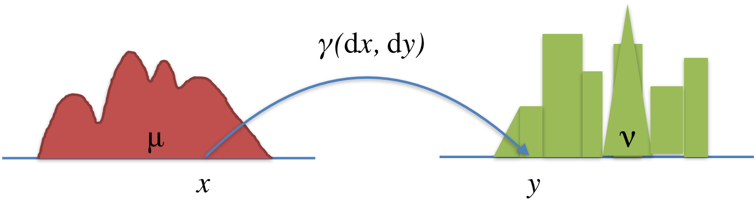

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- A transport plan (or coupling) between μ and ν is a probability measure $\gamma \in \mathcal{P}(\mathcal{X} \times \mathcal{X})$ s.t.

$$\gamma(A \times \mathcal{X}) = \mu(A) \quad \text{and} \quad \gamma(\mathcal{X} \times A) = \nu(A) \quad \forall A \subseteq \mathcal{X} \ .$$

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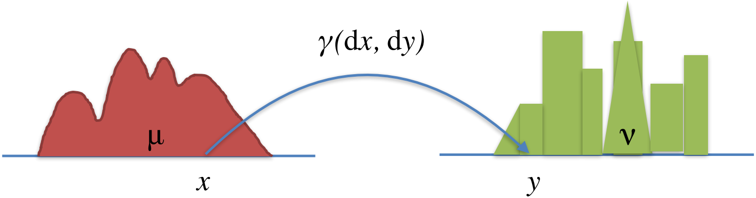

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The Monge-Kantorovich problem (1781, 1942)

Minimize $\gamma \mapsto \int_{\mathcal{X} \times \mathcal{X}} c(x, y) \, \mathrm{d}\gamma(x, y)$ among all $\gamma \in \mathrm{Cpl}(\mu, \nu)$.

Diffusion equations via optimal transport

Jordan–Kinderlehrer–Otto '98: Beautiful connection between

- the 2-Kantorovich metric on the space of probability measures

$$W_2(\mu, \nu) = \inf_{\gamma \in \mathsf{Cpl}(\mu,\nu)} \sqrt{\int_{\mathbb{R}^n \times \mathbb{R}^n} |x - y|^2 \, \mathrm{d}\gamma(x, y)}$$

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- the (negative of the) Boltzmann-Shannon entropy

$$\mathsf{Ent}(\mu) = \int_{\mathbb{R}^n} \rho(x) \log \rho(x) \, \mathrm{d}x, \qquad \text{if} \quad \mathrm{d}\mu(x) = \rho(x) \, \mathrm{d}x$$

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$$\partial_t \mu = \Delta \mu$$

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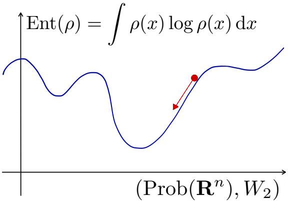
Theorem (J-K-O '98)

The heat flow is the gradient flow of the entropy w.r.t W_2.



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Gradient flows in $\mathbb{R}^n$

Let $\varphi : \mathbb{R}^n \to \mathbb{R}$ smooth and convex. For $u : \mathbb{R}_+ \to \mathbb{R}^n$ TFAE:

1. u solves the gradient flow equation $u'(t) = -\nabla\varphi(u(t))$.

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   $$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|u(t) - y|^2 = \big(u(t) - y\big) \cdot u'(t) \leq \varphi(y) - \varphi(u(t)) \qquad \forall y \; .$$

   (De Giorgi '93, Ambrosio–Gigli–Savaré '05)

Diffusion equations via optimal transport

Theorem (Jordan–Kinderlehrer–Otto '98)

The heat flow is the gradient flow of the entropy w.r.t W_2 , i.e.,

$$\partial_t \mu = \Delta \mu \quad \Longleftrightarrow \quad \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t} W_2(\mu_t, \nu)^2 \leq \mathrm{Ent}(\nu) - \mathrm{Ent}(\mu_t) \qquad \forall \nu \ .$$

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Gradient flows in R^n

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• $\mathbb{R}^n$	Jordan–Kinderlehrer–Otto
• Riemannian manifolds	Villani, Erbar
• Hilbert spaces	Ambrosio–Savaré–Zambotti
• Finsler spaces	Ohta–Sturm
• Wiener space	Fang–Shao–Sturm
• Heisenberg group	Juillet
• Alexandrov spaces	Gigli–Kuwada–Ohta
• Metric measures spaces	Ambrosio–Gigli–Savaré

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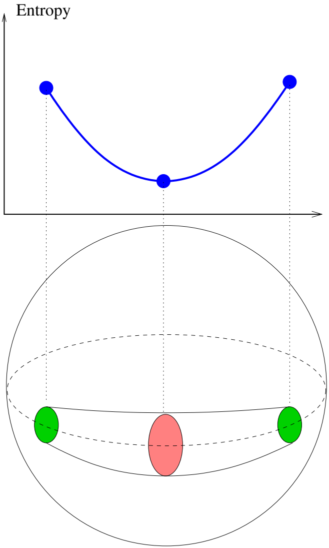
- is physically appealing
- comes with time-discrete approximation schemes
- applies to non-smooth problems
- yields functional inequalities and equilibration rates
- is closely connected to geometry (Ricci curvature)

Optimal transport and curvature

The "lazy gas experiment" (see VILLANI '09)



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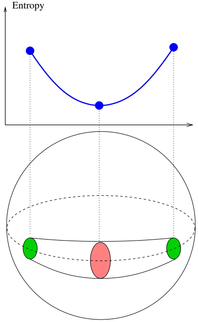
$$\mathrm{Ent}(\mu_t) \leq (1-t)\mathrm{Ent}(\mu_0) + t\mathrm{Ent}(\mu_1) - \frac{\kappa}{2} t(1-t) W_2^2(\mu_0, \mu_1)$$

for all W_2-geodesics $(\mu_t)_{t\in[0,1]}$ in $\mathcal{P}(\mathcal{M})$.



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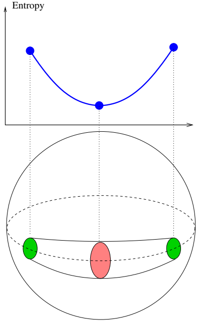

$\rightsquigarrow$ Ricci curvature in metric measure spaces (Lott–Sturm–Villani)

Ricci curvature via optimal transport

Definition (Sturm '06, Lott–Villani '09)

A metric measure space $(\mathcal{X}, d, m)$ satisfies $\mathrm{Ric}(\mathcal{X}) \geq \kappa$ if

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- Many geometric, analytic and probabilistic consequences
  $\longrightarrow$ logarithmic Sobolev, Talagrand, Poincaré inequalities; concentration of measure.
- Stability under measured Gromov–Hausdorff convergence

$\rightsquigarrow$ rich theory, very active research area

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Teaser: On the two point space: **Yes!**

$$\mathcal{W}(\mu_\alpha, \mu_\beta) = \int_\alpha^\beta \sqrt{\frac{\mathrm{arctanh}(2r-1)}{2r-1}} \, \mathrm{d}r, \qquad 0 \le \alpha \le \beta \le 1.$$

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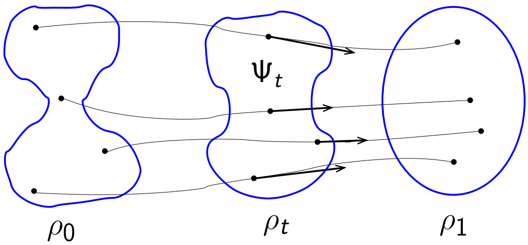
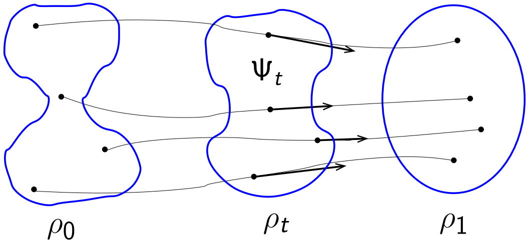


Back to R^n: dynamical characterisation of W_2

Benamou-Brenier formula in R^n

$$W_2(\rho_0,\rho_1)^2 = \inf_{(\rho_t,\Psi_t)_t} \left\{ \int_0^1 \int_{\mathsf{R}^n} |\Psi_t(x)|^2 \, \rho_t(x) \, \mathrm{d}x \, \mathrm{d}t \ : \ \partial_t \rho + \nabla \cdot (\rho \Psi) = 0 \ , \quad \rho|_{t=0} = \rho_0 \ , \quad \rho|_{t=1} = \rho_1 \right\} .$$



Back to $\mathbb{R}^n$: dynamical characterisation of W_2

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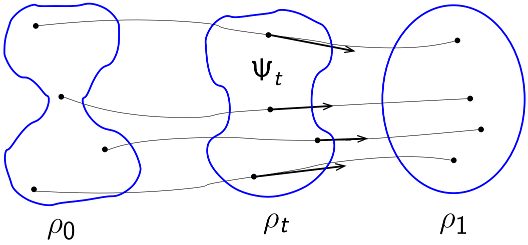
$$W_2(\rho_0,\rho_1)^2 = \inf_{(\rho_t,\psi_t)_t} \left\{ \int_0^1 \int_{\mathbb{R}^n} |\nabla \psi_t(x)|^2 \, \rho_t(x) \, \mathrm{d}x \, \mathrm{d}t \ : \right.$$

$$\partial_t \rho + \nabla \cdot (\rho \nabla \psi) = 0 \ ,$$

$$\left. \rho|_{t=0} = \rho_0 \ , \quad \rho|_{t=1} = \rho_1 \right\} .$$



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$$\mathcal{W}(\mu_0, \mu_1)^2$$

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Problem: μ is defined on vertices, $\nabla\psi$ is defined on edges.

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- Log-mean compensates for the lack of discrete chain rule:

$$\Lambda(\rho(x), \rho(y)) = \int_0^1 \rho(x)^{1-p} \rho(y)^p \, \mathrm{d}p = \frac{\rho(x) - \rho(y)}{\log \rho(x) - \log \rho(y)}$$

Ricci curvature of Markov chains

Definition (à la Lott–Sturm–Villani) (Erbar, M.)

A Markov chain $(\mathcal{X}, Q, \pi)$ is said to have Ricci curvature bounded from below by $\kappa \in \mathbb{R}$ if the relative entropy Ent_π is κ-convex along $\mathcal{W}$-geodesics.

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Simple examples with positive curvature

- discrete hypercube $\{-1, 1\}^n$: $\frac{2}{n}$
- Bernoulli-Laplace model (with k particles on n sites): $\frac{n+2}{k(n-k)}$
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Remark Many other notions of discrete Ricci curvature exist, e.g.:

- Ollivier's course Ricci curvature
- Bakry-Émery curvature (in various versions).

Consequences: Sharp functional inequalities

Bakry–Émery Theorem (Erbar, M.)

Let $(\mathcal{X}, Q, \pi)$ be a reversible Markov chain. Let $\kappa > 0$.

If $\mathrm{Ric}(K) \geq \kappa$, then the logarithmic Sobolev inequality holds:

$$\mathrm{Ent}_\pi(\rho\pi) \leq \frac{1}{2\kappa}\mathcal{E}(\rho, \log \rho) \,,$$

where $\mathcal{E}(\varphi, \psi) = -\langle \mathcal{L}\varphi, \psi \rangle_{L^2(\pi)}$ is the Dirichlet form.

This implies exponential decay of the relative entropy:

$$\mathrm{Ent}_\pi(e^{tL^\dagger}\mu) \leq e^{-2\kappa t}\,\mathrm{Ent}_\pi(\mu) \qquad \forall \mu \in \mathcal{P}(\mathcal{X}) \,.$$

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- Dissipative quantum mechanics (Carlen-M., Mielke-Mittnenzweig, Chen-Gangbo-Georgiou-Tannenbaum)
  non-commutative analogue of $\mathcal{W}$ for density matrices

Is there a JKO theorem for dissipative quantum systems?

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where the Hamiltonian H is self-adjoint, and $V_j \in B(\mathfrak{H})$.

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- H-Theorem [Spohn '78]: $t \mapsto \mathrm{Ent}(\mathcal{P}_t \rho|\sigma)$ is decreasing.

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- How to define the product $\bullet$?
  Need: non-commutative version of the classical chain rule

$$\nabla \rho = \rho \nabla \log \rho \ ?$$

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- Then: $\mathcal{L} = \sum_j e^{\omega_j/2} \mathcal{L}_j$, $\qquad \mathcal{L}_j \rho = [V_j, \rho V_j^*] + [V_j \rho, V_j^*]$, where $\{V_j\} = \{V_j^*\}$ and $[V_j, \log \sigma] = -\omega_j V_j$ for some $\omega_j \in \mathrm{R}$.

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- Then: $\mathcal{L} = \sum_j e^{\omega_j/2}\mathcal{L}_j$, $\qquad \mathcal{L}_j\rho = [V_j, \rho V_j^*] + [V_j\rho, V_j^*]$, where $\{V_j\} = \{V_j^*\}$ and $[V_j, \log\sigma] = -\omega_j V_j$ for some $\omega_j \in \mathrm{R}$.
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$$\sigma\nabla(\rho/\sigma) = \rho\nabla(\log\rho - \log\sigma)$$

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Quantum JKO-Theorem II (Carlen-M., Mielke-Mittnenzweig 2017)

If $\mathcal{L}$ satisfies detailed balance w.r.t. a state σ, then the Lindblad equation $\partial_t\rho = \mathcal{L}\rho$ is the gradient flow of the quantum relative entropy $\mathrm{Ent}(\rho|\sigma) = \mathrm{Tr}[\rho(\log\rho - \log\sigma)]$ w.r.t $\mathcal{W}$.

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- $\exists!$ (Gaussian) stationary state: $\sigma_\beta = Z^{-1} e^{-\beta H}$, $H = a^* a$

Theorem: [Carlen/M. '17]

$$\mathrm{Ent}(e^{t\mathcal{L}_\beta} \rho | \sigma_\beta) \leq e^{-2\lambda_\beta t}\, \mathrm{Ent}(\rho | \sigma_\beta) \quad \text{where} \quad \lambda_\beta = \sinh(\beta/2) \,.$$

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- Matrix convexity inequalities:

$$(R, A) \mapsto \mathrm{Tr}\left[\int_0^\infty (tI + e^{-\omega/2} R)^{-1} A^* (tI + e^{\omega/2} R)^{-1} A \, \mathrm{d}t \right]$$

  is jointly convex on $\mathcal{M}_n^+ \times \mathcal{M}_n$ for all $\omega \in \mathrm{R}$.

Thank you!