A gradient flow approach to chemical master equations

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Joint work with Alexander Mielke

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Starting point

Theorem (Jordan–Kinderlehrer–Otto '98)

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

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2011 – now: Related gradient flow structure have been found for

- discrete spaces / Markov chains
- reaction-diffusion systems
- dissipative quantum systems

New transportation metrics ($\neq W_2$) emerge!

W_2 as Riemannian metric (Otto '01)

- If $(\rho_t)_t$ is "nice", the continuity equation

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holds for some velocity vector field $\Psi(t, x)$.

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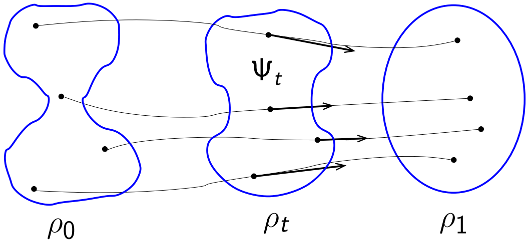

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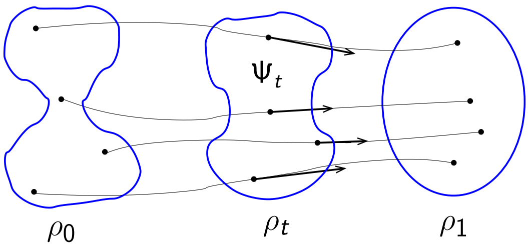

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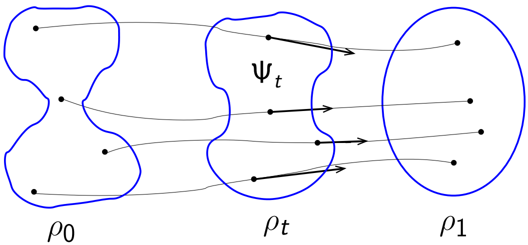

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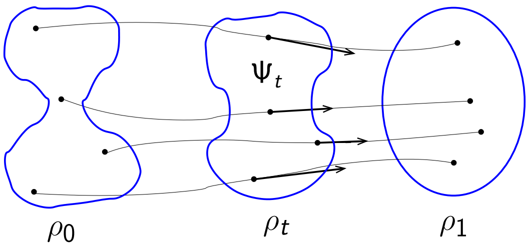

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Benamou-Brenier formula

$$W_2(\bar{\rho}_0, \bar{\rho}_1)^2 = \inf_{\rho_\cdot, \psi_\cdot} \left\{ \int_0^1 \|\nabla \psi_t\|_{\rho_t}^2 \, \mathrm{d}t \ : \partial_t \rho + \mathrm{div}(\rho \nabla \psi) = 0 \ , \quad \rho_0 = \bar{\rho}_0 \ , \quad \rho_1 = \bar{\rho}_1 \right\} .$$

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$\rightsquigarrow$ JKO-Theorem does not apply to discrete spaces.

Discrete setting

Setting

- $\mathcal{X}$: countable set
- $Q(x, y)$: transition rate from x to y
- π: reversible measure, $\quad \forall x, y \ : \ Q(x, y)\pi(x) = Q(y, x)\pi(y)$

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Heat flow

- Markov generator: $\Delta\psi(x) := \sum_y Q(x, y)(\psi(y) - \psi(x))$
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Relative Entropy

- $\mathcal{P}(\mathcal{X}) := \left\{ \rho : \mathcal{X} \to \mathbb{R}_+ \ \middle| \ \sum_{x\in\mathcal{X}} \rho(x)\pi(x) = 1 \right\}$
- $\mathrm{Ent}(\rho) := \sum_{x\in\mathcal{X}} \rho(x) \log \rho(x)\, \pi(x) \ , \qquad \rho \in \mathcal{P}(\mathcal{X})\ .$

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What about the general discrete case?

Definition of the metric $\mathcal{W}$

Benamou-Brenier formula in $\mathbb{R}^n$

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

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$$\mathcal{W}(\rho_0, \rho_1)^2$$

$$:= \inf_{\rho,\psi} \left\{ \int_0^1 \sum_{x,y \in \mathcal{X}} (\psi_t(x) - \psi_t(y))^2 \qquad Q(x,y)\pi(x) \, \mathrm{d}t \right\}$$

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Problem: $\rho(x)$ is defined on vertices, $\nabla\psi(x,y)$ is defined on edges

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Use the *logarithmic mean* as the "density on an edge"!

$$\hat{\rho}(x,y) := \int_0^1 \rho(x)^{1-\alpha} \rho(y)^{\alpha} \, \mathrm{d}\alpha = \frac{\rho(x) - \rho(y)}{\log \rho(x) - \log \rho(y)}$$

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- Represent heat equation as continuity equation:

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

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Discrete curvature and functional inequalities

Discrete analogue of Lott–Sturm–Villani:

Definition (Discrete Ricci lower bound)

Let $\kappa \in \mathbb{R}$. We say that $Ric(\mathcal{X}, Q, \pi) \geq \kappa$ if
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Many other approaches to Ricci curvature of discrete spaces:

- Ollivier, Joulin
- Bonciocat, Sturm
- Li, S.-T. Yau
- Gozlan, Roberto, Samson, Tetali
- Léonard
- Hillion
- ...

Consequences: Sharp functional inequalities

Theorem (Erbar, M.)

Let $(\mathcal{X}, Q, \pi)$ be a reversible Markov chain. Let $\kappa > 0$.
Set $\mathcal{E}(\varphi, \psi) = \frac{1}{2} \sum_{x,y} (\varphi(x) - \varphi(y))(\psi(x) - \psi(y)) Q(x, y) \pi(x)$.

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$$\mathrm{Ent}(\rho) \leq \frac{1}{2\kappa}\mathcal{E}(\rho, \log \rho) \qquad \forall \rho \ .$$

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3. Talagrand ineq $\implies$ Poincaré inequality, i.e.,

$$\|\varphi\|^2_{L^2(\mathcal{X},\pi)} \;\leq\; \frac{1}{\kappa}\mathcal{E}(\varphi, \varphi) \qquad \forall \psi \,.$$

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2. Geodesic convexity of the Boltzmann entropy along $\mathcal{W}_\alpha$-geodesics.

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- $f : [0, \infty) \to \mathbb{R}$ strictly convex.
  $\rightsquigarrow$ generalised entropy:

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Discrete porous medium equations

- $\varphi : [0,\infty) \to \mathbb{R}$ strictly increasing.
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Theorem (Erbar, M. '12)

The discrete PME is the gradient flow of $\mathcal{F}$ w.r.t. $\mathcal{W}$, provided that

$$\hat\rho(x,y) = \theta\big(\rho(x),\rho(y)\big)\ , \qquad \text{with} \qquad \theta(r,s) = \frac{\varphi(r)-\varphi(s)}{f'(r)-f'(s)}\ .$$

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- Special case: $\varphi(r) = r^m$ and $f(r) = \frac{1}{m-1} r^m$. Then:

$$\theta_m(r,s) = \frac{m-1}{m} \frac{r^m - s^m}{r^{m-1} - s^{m-1}} \ .$$

Chemical reaction networks

Consider K chemical species $X_1, \ldots, X_K$ subject to R reversible reactions:

$$\alpha_1^r X_1 + \cdots + \alpha_K^r X_K \underset{k_{\mathrm{fw}}^r}{\overset{k_{\mathrm{bw}}^r}{\rightleftharpoons}} \beta_1^r X_1 + \cdots + \beta_K^r X_K$$

for $r = 1, \ldots, R$.

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We consider 2 well-known mathematical models:

- deterministic ODE model
- stochastic Markov chain model

The deterministic model

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- Observable: $\mathbf{c} = (c_1, \ldots, c_K) \in \mathbb{R}_+^K$: concentration of species $X_1, \ldots, X_K$.

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- Time-evolution: reaction rate equation (RRE)

$$\dot{\mathbf{c}} = -\mathbf{R}(\mathbf{c}) \quad \text{with } \mathbf{R}(\mathbf{c}) := \sum_{r=1}^{R} \left(k_{\mathrm{fw}}^r \mathbf{c}^{\boldsymbol{\alpha}^r} - k_{\mathrm{bw}}^r \mathbf{c}^{\boldsymbol{\beta}^r}\right)\Big(\boldsymbol{\alpha}^r - \boldsymbol{\beta}^r\Big)$$

where $\mathbf{c}^{\boldsymbol{\alpha}} = \prod_{k=1}^{K} c_k^{\alpha_k}$.

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  where $\mathbf{c}^{\boldsymbol{\alpha}} = \prod_{k=1}^{K} c_k^{\alpha_k}$.
- Standing assumption: detailed balance (DB): there exists $\mathbf{c}_* \in \mathbb{R}_{>0}^K$ such that

$$k_{\mathrm{fw}}^r \mathbf{c}_*^{\boldsymbol{\alpha}^r} = k_{\mathrm{bw}}^r \mathbf{c}_*^{\boldsymbol{\beta}^r} =: \kappa_r \qquad \text{for all } r = 1, \ldots, R$$

Gradient flow structure for RRE

Gradient flow structure for RRE (Mielke '11)

Assume that $\mathbf{c}_* \in \mathbb{R}^K_{>0}$ satisfies detailed balance. Then, the RRE is the gradient flow of the relative entropy E in $(\mathbb{R}^K_+, d_{RRE})$, where

$$E(\mathbf{c}) = \sum_{k=1}^{K} c_k^* \lambda_{\mathrm{B}}\big(\tfrac{c_k}{c_k^*}\big) \quad \text{and} \quad \lambda_{\mathrm{B}}(t) := t \log t - t + 1 \ ,$$

$$d_{RRE}(\mathbf{c}_0, \mathbf{c}_1)^2 := \inf_{\mathbf{c},\boldsymbol{\xi}} \Big\{ \int_{s=0}^{1} \sum_{r=1}^{R} \kappa_r \, \mu_r(\mathbf{c}(s)) \, \langle \boldsymbol{\xi}(s), \gamma^r \rangle^2 \, \mathrm{d}s \ : \ \dot{\mathbf{c}}(s) = \sum_{r=1}^{R} \kappa_r \, \mu_r(\mathbf{c}(s)) \, \langle \boldsymbol{\xi}(s), \gamma^r \rangle \gamma^r \Big\} \ ,$$

with mobility

$$\mu_r(\mathbf{c}) := \Lambda\left(\frac{\mathbf{c}^{\boldsymbol{\alpha}^r}}{\mathbf{c}_*^{\boldsymbol{\alpha}^r}}, \frac{\mathbf{c}^{\boldsymbol{\beta}^r}}{\mathbf{c}_*^{\boldsymbol{\beta}^r}} \right) \ , \qquad \Lambda(a,b) := \int_0^1 a^{1-r} b^r \, \mathrm{d}r \ .$$

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	Transition	Rate
fw	$\mathbf{n} \to \mathbf{n} + (\boldsymbol{\beta}^r - \boldsymbol{\alpha}^r)$	$k_{\mathrm{fw}}^r \, \mathbb{B}_V^{\boldsymbol{\alpha}^r}(\mathbf{n})$
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$$\mathbb{B}_V^{\boldsymbol{\alpha}}(\mathbf{n}) = \frac{1}{V^{|\boldsymbol{\alpha}|-1}} \prod_{k=1}^{K} \frac{n_k!}{(n_k - \alpha_k)!} \mathbf{1}_{\{n_k \geq \alpha_k\}} , \qquad V > 0 \text{ (volume)}$$

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- Let $u_V(t) \in \mathrm{Prob}(\mathbb{N}_0^K)$ be the distribution of $\mathbf{Y}(t)$.

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- Let $u_V(t) \in \mathrm{Prob}(\mathbb{N}_0^K)$ be the distribution of $\mathbf{Y}(t)$.
- $u_V(t)$ evolves according to the chemical master equation.

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- If $\mathbf{c}_* \in \mathbb{R}^K_{>0}$ satisfies detailed balance for the RRE, then the measure $\mathbf{w}^V \in \mathrm{Prob}(\mathbb{N}_0^K)$ given by

$$w_{\mathbf{n}}^V = \frac{1}{Z_V} \frac{V^{|\mathbf{n}|}\mathbf{c}_*^{\mathbf{n}}}{\mathbf{n}!}$$

  satisfies the detailed balance condition for CME.

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Consequently:

Gradient flow structure for CME

The CME is the gradient flow of the relative entropy $\mathrm{Ent}(\cdot|\mathbf{w}^V)$ w.r.t. a discrete transportation metric.

Gradient flows for CME and RRE

Two gradient flow structures:

- the RRE $\dot{\mathbf{c}} = -\mathbf{R}(\mathbf{c})$ is the gradient flow of $E = \mathrm{Ent}(\cdot|\mathbf{c}_*)$
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Can we interpret this at the level of the gradient structures?

Passing to the limit: the entropy

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- Rescaled entropy for CME:

$$\frac{1}{V}\,\mathrm{Ent}(\mathbf{u}|\mathbf{w}^V) = \frac{1}{V}\sum_{\mathbf{n}\in\mathcal{N}} u_{\mathbf{n}} \log u_{\mathbf{n}} - \frac{1}{V}\sum_{\mathbf{n}\in\mathcal{N}} u_{\mathbf{n}} \log w^V_{\mathbf{n}}$$

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- Second term: Stirling's formula yields

$$-\frac{1}{V}\log w^V_{\mathbf{n}} \approx E\Big(\frac{\mathbf{n}}{V}\Big)\,,$$

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hence

$$\frac{1}{V}\,\mathrm{Ent}(\mathbf{u}|\mathbf{w}^V) \approx \sum_{\mathbf{n}\in\mathbb{N}_0^K} u_{\mathbf{n}} E(\frac{\mathbf{n}}{V}) \to \int_{\mathbb{R}_+^K} E(\mathbf{c})\,\mathrm{d}\rho(\mathbf{c}).$$

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- Dual dissipation functional for CME: $\Psi^*_V(\mathbf{u},\psi) =$

$$V\sum_{\mathbf{n},r}\kappa^r_*\,(\psi_{\mathbf{n}+\boldsymbol{\gamma}^r}-\psi_{\mathbf{n}})^2\,\Lambda\Bigg(\frac{\mathbb{B}_V^{\boldsymbol{\alpha}^r}(\mathbf{n}+\boldsymbol{\gamma}^r)}{\mathbf{c}_*^{\boldsymbol{\alpha}^r}}u_{\mathbf{n}+\boldsymbol{\gamma}^r},\,\frac{\mathbb{B}_V^{\boldsymbol{\beta}^r}(\mathbf{n})}{\mathbf{c}_*^{\boldsymbol{\beta}^r}}u_{\mathbf{n}}\Bigg).$$

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Ψ^* is the action functional in the Benamou-Brenier formulation of the W_2-metric induced by d_{RRE}.

The Liouville equation

Theorem (M., Mielke)

We have convergence of the gradient flow structure:

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What is the gradient flow equation of the limit $(\mathbf{E}, W_2^{\mathsf{RRE}})$?

The Liouville equation

Theorem (M., Mielke)

We have convergence of the gradient flow structure:

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The grad. flow equation of $\mathbf{E}$ w.r.t. W_2^{RRE} is the Liouville equation

$$\partial_t \rho_t(\mathbf{c}) = \operatorname{div}(\rho_t(\mathbf{c})\mathbf{R}(\mathbf{c}))$$

where $\dot{\mathbf{c}} = -\mathbf{R}(\mathbf{c})$ is the reaction rate equation.

A Fokker-Planck approximation to the CME

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Rescaled entropy for CME:

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$$\mathbf{E}_V(\rho) = \mathbf{E}(\rho) + \tfrac{1}{V}\int \rho(\mathbf{c})\log\rho(\mathbf{c})\,\mathrm{d}\mathbf{c} + \int F_V(\mathbf{c})\,\mathrm{d}\rho(\mathbf{c}).$$

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The grad. flow eq. of $\mathbf{E}$ w.r.t. W_2^{RRE} is the Fokker-Planck equation

$$\dot\rho = \mathrm{div}\Big(\tfrac{1}{V}\mathbb{K}(\mathbf{c})\nabla\rho(\mathbf{c}) + \rho(\mathbf{c})\mathbf{R}(\mathbf{c}) + \rho(\mathbf{c})\mathbb{K}(\mathbf{c})\mathrm{D}F_V(\mathbf{c})\Big).$$

Thank you!