

## Discrete gradient flow structures for mean-field systems

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joint work with M. Erbar (U Bonn), M. Fathi (UC Berkeley) and V. Laschos (WIAS Berlin)

**YEP XIII Large deviations for interacting particle systems and PDEs, Eindhoven**



- $\mathcal{X}$  a finite set
- $N$  particles on  $\mathcal{X}$  distributed according to a **Gibbs measure**  $\pi \in \mathcal{P}(\mathcal{X}^N)$

$$\mathbf{x} \in \mathcal{X}^N : \quad \pi(\mathbf{x}) := \frac{1}{Z^N} \exp\left(-U^N(\mathbf{x})\right)$$

- Hamiltonian  $U^N : \mathcal{X}^N \rightarrow \mathbf{R}$  of **mean-field type**:  $\exists U : \mathcal{P}(\mathcal{X}) \rightarrow \mathbf{R}$

$$U^N(\mathbf{x}) = NU\left(L^N(\mathbf{x})\right) \quad \text{with} \quad L^N(\mathbf{x}) := \frac{1}{N} \sum_{i=1}^N \delta_{x_i}$$

- Example

$$U^N(\mathbf{x}) = \sum_{i=1}^N V(x_i) + \frac{1}{N} \sum_{i,j=1}^N W(x_i, x_j)$$

In terms of  $U$

$$U(\mu) = \sum_{x \in \mathcal{X}} \mu_x K_x(\mu) \quad \text{with} \quad K_x(\mu) = V(x) + \sum_{y \in \mathcal{X}} W(x, y) \mu_y$$

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Introduce a **reversible** dynamic wrt. Gibbs distribution  $\pi$

- Single particle jumps

$$\mathbf{x}^{i;y} := \mathbf{x} - (x_i - y)\mathbf{e}^i = (x_1, \dots, x_{i-1}, y, x_{i+1}, \dots, x_N).$$

- On the level of **empirical** distributions

$$\text{if } L^N(\mathbf{x}) = \nu \in \mathcal{P}_N(\mathcal{X}) \quad \text{then} \quad L^N(\mathbf{x}^{i;y}) = \nu^{N;x_i,y} := \nu - \frac{1}{N}(\delta_{x_i} - \delta_y)$$

- Make dynamic reversible wrt.  $\pi$

$$Q^N(\mathbf{x}, \mathbf{x}^{i;y}) = \sqrt{\frac{\pi_{\mathbf{x}^{i;y}}}{\pi_{\mathbf{x}}}} A_{x_i,y}^N(L^N(\mathbf{x})s) = Q^N(L^N(\mathbf{x}); x_i, y)$$

and  $\{A_{x,y}^N(\mu)\}_{\mu \in \mathcal{P}(\mathcal{X})}$  a family of irreducible symmetric matrices.

- Generator

$$\mathcal{L}^N f := \sum_{i=1}^N \sum_{y \in \mathcal{X}} (f(\mathbf{x}^{i;y}) - f(\mathbf{x})) Q_{\mathbf{x}, \mathbf{x}^{i;y}}^N.$$

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- Free energy for  $\mu^N \in \mathcal{P}(\mathcal{X}^N)$

$$\mathcal{F}^N(\mu) := \mathcal{H}^N(\mu | \pi) = \sum_{x \in \mathcal{X}^N} \mu_x \log \frac{\mu_x}{\pi_x}.$$

- Action of  $\mu \in \mathcal{P}(\mathcal{X}^N)$  and  $\psi \in \mathbf{R}^{\mathcal{X}^N}$

$$\mathcal{A}^N(\mu, \psi) = \frac{1}{2} \sum_{x, y} (\psi_y - \psi_x)^2 w_{x, y}^N(\mu) = \langle \psi, \mathcal{K}^N(\mu)\psi \rangle$$

with weights  $w_{x, y}^N(\mu)$  defined with  $\Lambda(a, b) = (a - b)/(\log a - \log b)$  as follows

$$w_{x, y}^N(\mu) := \Lambda\left(\mu_x Q^N(x, y), \mu_y Q^N(y, x)\right) = \Lambda\left(\frac{\mu_x}{\pi_x}, \frac{\mu_y}{\pi_y}\right) Q^N(x, y) \pi_x.$$

- Metric  $\mathcal{W}^N$  on  $\mathcal{P}(\mathcal{X}^N)$

$$\mathcal{W}^N(\mu, \nu)^2 := \inf_{(c, \psi)} \int_0^1 \mathcal{A}^N(c(t), \psi(t)) dt$$

with the infimum among pairs such that  $c(0) = \mu$ ,  $c(1) = \nu$  and

$$\dot{c}_x(t) + \sum_y (\psi_y(t) - \psi_x(t)) w_{x, y}^N(c(t)) = 0 \quad \Leftrightarrow \quad \dot{c}(t) = \mathcal{K}^N(c(t))\psi.$$

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- $N$ -particle Fisher information

$$\mathcal{I}^N(\mu) := \frac{1}{2} \sum_{(x, y) \in E_\mu} w_{x, y}^N(\mu) \left( \log(\mu_x Q^N(x, y)) - \log(\mu_y Q^N(y, x)) \right)^2$$

The evolution of the density  $c \in \mathcal{P}(\mathcal{X}^N)$  satisfies

$$\dot{c}_x(t) = \sum_y (c_y(t) Q_{y,x} - c_x(t) Q_{x,y}) = (c(t) Q)_x = - \left( \mathcal{K}^N(c(t)) D\mathcal{F}^N(c(t)) \right)_x.$$

The results of [Maas / Mielke, 2011] show that  $c$  is the gradient flow of  $\mathcal{F}^N$  wrt.  $\mathcal{W}^N$ .

### Proposition (Curves of maximal slope)

For  $c \in \text{AC}([0, T], (\mathcal{P}(\mathcal{X}^N), \mathcal{W}^N))$  the function  $\mathcal{J}^N$  given by

$$\mathcal{J}^N(c) := \mathcal{F}^N(c(T)) - \mathcal{F}^N(c(0)) + \frac{1}{2} \int_0^T \mathcal{I}^N(c(t)) dt + \frac{1}{2} \int_0^T \mathcal{A}^N(c(t), \psi(t)) dt,$$

is non-negative, where  $\psi_t$  is such that the continuity equation holds. Moreover, a curve  $c$  is a solution to  $\dot{c}(t) = c(t) Q^N$  if and only if  $\mathcal{J}^N(c) = 0$ .

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$$\pi_x(\mu) = \frac{1}{Z(\mu)} \exp(-H_x(\mu)), \quad \text{with } H_x(\mu) = \frac{\partial}{\partial \mu_x} U(\mu), \quad \text{and } U(\mu) = \sum_{x \in \mathcal{X}} \mu_x K_x(\mu).$$

- $Q(\mu)$  reversible rates wrt.  $\pi(\mu)$

$$Q_{xy}(\mu) = \sqrt{\frac{\pi_y(\mu)}{\pi_x(\mu)}} A_{xy}(\mu) \quad \text{with } A(\mu) \in \mathbf{R}^{\mathcal{X} \times \mathcal{X}} \text{ irreducible and symmetric.}$$

- nonlinear ODE for  $c \in C^1([0, T], \mathcal{P}(\mathcal{X}))$

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$$\mu \mapsto \pi(\mu) : \quad \pi(\pi^*) = \pi^*.$$

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Free energy  $\mathcal{F} : \mathcal{P}(\mathcal{X}) \rightarrow \mathbf{R}$

$$\mathcal{F}(\mu) = \sum_{x \in \mathcal{X}} \mu_x \log \mu_x + U(\mu).$$

Note:  $\mathcal{F}(\mu) \neq \mathcal{H}(\mu \mid \pi(\mu))$ . However  $\partial_{\mu_x} \mathcal{F}(\mu) = \log \frac{\mu_x}{\pi_x(\mu)} + 1 - \log Z(\mu)$ .

Onsager operator  $\mathcal{K} : \mathbf{R}^{\mathcal{X}} \rightarrow \mathbf{R}^{\mathcal{X}}$  defined for  $\psi \in \mathbf{R}^{\mathcal{X}}$  by

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### Formal gradient flow

$$\dot{c}(t) = -\mathcal{K}(c(t))D\mathcal{F}(c(t)).$$

Dissipation:

$$\frac{d}{dt} \mathcal{F}(c(t)) = -\mathcal{I}(c(t)) = -\frac{1}{2} \sum_{x,y} w_{xy}(c) (\log(c_x Q_{xy}(c)) - \log(c_y Q_{yx}(c)))^2.$$



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### Proposition (Metric)

The space  $(\mathcal{P}(\mathcal{X}), \mathcal{W})$  with the metric defined by

$$\mu, \nu \in \mathcal{P}(\mathcal{X}) : \quad \mathcal{W}^2(\mu, \nu) := \inf_{(c, \psi)} \left\{ \int_0^1 \mathcal{A}(c(t), \psi(t)) dt \right\},$$

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is a complete separable metric space.

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### Proposition (Curves of maximal slope)

For any  $(c(t))_{t \in [0, T]} \in \text{AC}([0, T], (\mathcal{P}(\mathcal{X}), \mathcal{W}))$  holds

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Moreover,  $\mathcal{J}(c) = 0$  if and only if  $\dot{c} = cQ(c)$ . In this case  $c(t) \in \mathcal{P}^*(\mathcal{X})$  for all  $t > 0$ .

- Since  $L_{\sharp}^N \mu^N \in \mathcal{P}(\mathcal{P}_N(\mathcal{X}))$ , a **lifting** of the ODE from  $\mathcal{P}(\mathcal{X})$  to  $\mathcal{P}(\mathcal{P}(\mathcal{X}))$  is necessary to make it compatible
- For randomized initial data law  $c(0) = \mathbb{C}(0) \in \mathcal{P}(\mathcal{P}(\mathcal{X}))$  holds

$$\partial_t \mathbb{C}(t, c) + \operatorname{div}_{\mathcal{P}(\mathcal{X})} (\mathbb{C}(t, c) c Q(c)) = 0. \quad (\text{Lio})$$

- free energy  $\mathbb{F}$ , action  $\mathbb{A}$ , Fisher information  $\mathbb{I}$  are defined as averages of their unlifted counterparts:

$$\mathbb{F}(\mathbb{C}) := \int \mathcal{F}(\nu) \mathbb{C}(d\nu).$$

- Consistency of definition of metric

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Master equation $\mathbf{X}_t^N$ Markov $(\mathcal{L}^N, \mathcal{X}^N)$	$\mathbf{c} \in \text{AC}([0, t], (\mathcal{P}(\mathcal{X}^N), \mathcal{W}^N))$
$\dot{\mathbf{c}}(t) = -\mathcal{K}^N(\mathbf{c}(t))D\mathcal{H}^N(\mathbf{c}(t)   \boldsymbol{\pi})$	$\stackrel{\text{de Giorgi}}{\iff} \mathcal{J}^N(\mathbf{c}) = 0$
$\Downarrow L_{\#}^N$	$\Downarrow L_{\#}^N$
$\mathbb{C}^N$ Markov $(\bar{\mathcal{L}}^N, \mathcal{P}_N(\mathcal{X}))$	$\mathbb{C}^N \in \text{AC}([0, T], (\mathcal{P}(\mathcal{P}_N(\mathcal{X})), \mathcal{W}^N))$
$\Downarrow N \rightarrow \infty$	$\Downarrow N \rightarrow \infty$
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Proof  $\Gamma$ -lim inf estimate for  $\mathcal{J}^N$  wrt.  $\mathbb{J}$ , whenever  $L_{\#}^N \mathbf{c} \xrightarrow{d} \mathbb{C}$  on  $[0, T]$

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### Theorem (Sandier-Serfaty)

Assume that whenever a sequence  $c^N \in AC([0, T], (\mathcal{P}(\mathcal{X}^N), \mathcal{W}^N))$  for  $t \in [0, T]$  it holds  $L_{\#}^N c^N(t) \xrightarrow{d} \mathbb{C}(t) \in \mathcal{P}(\mathcal{P}(\mathcal{X}))$  and

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In addition, assume it holds

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### Proposition ( $\liminf$ -estimate for free energy)

If  $L_{\sharp}^N \mu^N \xrightarrow{d} \mathbb{M}$ , then

$$\lim_{N \rightarrow \infty} \frac{1}{N} \mathcal{H}(\mu^N \mid \pi) \geq \int_{\mathcal{P}(\mathcal{X})} (\mathcal{F}(\nu) - \mathcal{F}_0) \mathbb{M}(d\nu) = \mathbb{F}(\mathbb{M}) - \mathcal{F}_0, \quad (\text{A0})$$

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**Proof:** Decompose relative entropy

$$\frac{1}{N} \mathcal{H}(\mu^N | \pi^N) = \frac{1}{N} \mathcal{H}(\mu^N) + \mathbb{E}_{L_{\#}^N \mu^N} [U] + \frac{1}{N} \log \mathbf{Z}^N$$

Decompose entropy by using  $\mathcal{T}_N(\nu) = \{\mathbf{x} \in \mathcal{X}^N : L^N(\mathbf{x}) = \nu\}$

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$$\frac{1}{N} \mathcal{H}(\mu^N | \pi^N) = \frac{1}{N} \mathcal{H}(\mu^N) + \mathbb{E}_{L_{\#}^N \mu^N} [U] + \frac{1}{N} \log \mathbf{Z}^N$$

Decompose entropy by using  $\mathcal{T}_N(\nu) = \{\mathbf{x} \in \mathcal{X}^N : L^N(\mathbf{x}) = \nu\}$

$$\frac{1}{N} \mathcal{H}(\mu^N) \geq -\frac{1}{N} \log |\mathcal{P}_N(\mathcal{X})| - \frac{1}{N} \mathbb{E}_{L_{\#}^N \mu^N} [\log |\mathcal{T}_N|]$$

$$\text{Stirling} \geq -\frac{d \log N}{N} + \mathbb{E}_{L_{\#}^N \mu^N} [\mathcal{H}_{\mathcal{P}(\mathcal{X})}(\bullet)] - \frac{\log(N+1)}{N}$$

### Proposition (lim inf-estimate for free energy)

If  $L_{\#}^N \mu^N \xrightarrow{d} \mathbb{M}$ , then

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By Sanov's Theorem:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \log \mathbf{Z}^N = - \inf_{\nu \in \mathcal{P}(\mathcal{X})} \left\{ \sum_{x \in \mathcal{X}} \nu(x) \log \nu(x) + U(\nu) \right\} =: -\mathcal{F}_0.$$



### Proposition (Convergence of metric derivative and slopes)

Let  $\mathbf{c}^N \in \text{AC}([0, T], (\mathcal{P}(\mathcal{X}^N), \mathcal{W}^N))$  with  $(\mathbf{c}^N, \boldsymbol{\psi}^N)$  solving the continuity equation.  
If

$$L_{\#}^N \mathbf{c}^N \xrightarrow{d} \mathbb{C} \quad \text{for some measurable } \mathbb{C} : [0, T] \rightarrow \mathcal{P}(\mathcal{P}(\mathcal{X})),$$

such that

$$\limsup_{N \rightarrow \infty} \int_0^T \frac{1}{N} \mathcal{A}^N(\mathbf{c}^N(t), \boldsymbol{\psi}^N(t)) dt < \infty.$$

Then  $\mathbb{C} \in \text{AC}([0, T], \mathcal{P}(\mathcal{P}(\mathcal{X})))$ , and it exists  $\Psi : [0, T] \times \mathcal{P}(\mathcal{X}) \rightarrow \mathbf{R}^X$ , for which  $(\mathbb{C}, \Psi)$  solves the continuity equation and it holds

$$\liminf_{N \rightarrow \infty} \int_0^T \frac{1}{N} \mathcal{A}^N(\mathbf{c}^N(t), \boldsymbol{\psi}^N(t)) dt \geq \int_0^T \mathbb{A}(\mathbb{C}(t), \Psi(t)) dt \quad (\text{A1})$$

and

$$\liminf_{N \rightarrow \infty} \int_0^T \frac{1}{N} \mathcal{I}^N(\mathbf{c}^N(t)) dt \geq \int_0^T \mathbb{I}(\mathbb{C}(t)) dt. \quad (\text{A2})$$

Previous results + tightness for particle system imply:

### Theorem (Convergence of the particle system to the mean field equation)

Let  $\mathbf{c}^N$  be the law of the  $N$ -particle system. Moreover assume its initial distribution to be well prepared

$$\frac{1}{N} \mathcal{F}^N(\mathbf{c}^N(0)) \rightarrow \mathbb{F}(\mathbb{C}(0)) - \mathcal{F}_0 \quad \text{with} \quad L_{\sharp}^N \mathbf{c}^N(0) \xrightarrow{d} \mathbb{C}(0) \quad \text{as } N \rightarrow \infty.$$

Then it holds

$$L_{\sharp}^N \mathbf{c}^N(t) \xrightarrow{d} \mathbb{C}(t) \quad \text{for all } t \in (0, \infty),$$

with  $\mathbb{C}$  a weak solution to (Lio) and moreover

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Similar results in this spirit:

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### Definition ( $\kappa$ -convexity wrt. $\mathcal{W}$ )

$\{Q(\mu) \in \mathcal{R}^{\mathcal{X} \times \mathcal{X}}\}_{\mu \in \mathcal{P}(\mathcal{X})}$  is  $\kappa$ -convex with  $\kappa \in \mathbf{R}$ , if for any constant speed geodesic  $c \in \text{AC}([0, 1], (\mathcal{P}(\mathcal{X}), \mathcal{W}))$  holds

$$\mathcal{F}(c(t)) \leq (1-t)\mathcal{F}(c(0)) + t\mathcal{F}(c(1)) - \kappa \frac{t(1-t)}{2} \mathcal{W}^2(c(0), c(1)).$$

### Corollary (Two-point space)

Assume  $\mathcal{X} = \{0, 1\}$ ,  $p(\mu) := Q(\mu; 0, 1)$  and  $q(\mu) := Q(\mu; 1, 0)$  as well as  $p'(\mu) = \partial_{\mu_0} p(\mu)$  and  $q'(\mu) = \partial_{\mu_1} q(\mu)$  then the  $\kappa$  is give by

$$\kappa = \inf_{\mu \in \mathcal{P}(\mathcal{X})} \left( \frac{p(\mu) + q(\mu)}{2} + 3(\mu(0)p'(\mu) + \mu(1)q'(\mu)) \right. \\ \left. + \Lambda(\mu_0 p(\mu), \mu_1 q(\mu)) \left( \frac{1}{2\mu(0)p(\mu)} + \frac{1}{2\mu(1)q(\mu)} - \frac{p'(\mu)}{p(\mu)} - \frac{q'(\mu)}{q(\mu)} \right) \right).$$

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Mean-field Ising model on  $\mathcal{X} = \{0, 1\}$ . Define potentials by

$V(0) = V(1) = W(0, 0) = W(1, 1) = 0$  and  $W(0, 1) = W(1, 0) = \beta > 0$ . Hence  $K_0(\mu) = \beta\mu_1$ ,  $K_1(\mu) = \beta\mu_0$  and so

$$\mathcal{F}(\mu) = \sum_{\sigma \in \{0,1\}} (\log \mu_\sigma + K_\sigma(\mu)) \mu_\sigma = \mu_0 \log \mu_0 + \mu_1 \log \mu_1 + 2\beta\mu_0\mu_1.$$

As a function  $\mathcal{F} : \mathcal{P}(\mathcal{X}) \rightarrow \mathbf{R}$  is convex for  $\beta \leq 1$ .

Does the same holds for  $\kappa$ -convexity wrt.  $\mathcal{W}$ ?

For the dynamic use for instance Metropolis rates:

$$p_{\text{MC}}(\mu) = \exp(-2\beta(\mu(0) - \mu(1))_+) \quad q_{\text{MC}}(\mu) = \exp(-2\beta(\mu(1) - \mu(0))_+)$$

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### $\kappa$ -convexity.

- Proof lower bound in  $\kappa_{MC}(\beta) = 2 - 2\beta$
- Connect  $\kappa^N$ -convexity of  $N$ -particle system with  $\kappa$ -convexity of limit system:  
Easy:

$$\lim_{N \rightarrow \infty} \kappa^N \leq \kappa$$

Hard: Quantified comparison

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### Passage to the Limit.

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 $\Rightarrow$  Fokker-Planck equation
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