Discrete gradient flow structures for mean-field systems

André Schlichting

Institute for Applied Mathematics, University of Bonn

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

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Weakly interacting particle systems – Gibbs measure

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

$$\boldsymbol{x} \in \mathcal{X}^N : \qquad \boldsymbol{\pi}(\boldsymbol{x}) := \frac{1}{\boldsymbol{Z}^N} \exp\Big(-U^N(\boldsymbol{x})\Big)$$

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

$$U^N(\boldsymbol{x}) = NU\Big(L^N(\boldsymbol{x})\Big) \qquad \text{with} \qquad L^N(\boldsymbol{x}) := \frac{1}{N}\sum_{i=1}^N \delta_{x_i}$$

- Example

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

In terms of U

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

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Weakly interacting particle systems – Dynamics

Introduce a reversible dynamic wrt. Gibbs distribution $\boldsymbol{\pi}$

- Single particle jumps

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

- On the level of empirical distributions

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

- Make dynamic reversible wrt. π

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

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

- Generator

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

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

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

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

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

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

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

- 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

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

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- N-particle Fisher information

$$\boldsymbol{\mathcal{I}}^N(\boldsymbol{\mu}) := \frac{1}{2} \sum_{(\boldsymbol{x},\boldsymbol{y})\in E_{\boldsymbol{\mu}}} \boldsymbol{w}^N_{\boldsymbol{x},\boldsymbol{y}}(\boldsymbol{\mu}) \left(\log(\boldsymbol{\mu}_{\boldsymbol{x}} \boldsymbol{Q}^N(\boldsymbol{x},\boldsymbol{y})) - \log(\boldsymbol{\mu}_{\boldsymbol{y}} \boldsymbol{Q}^N(\boldsymbol{y},\boldsymbol{x}))\right)^2$$

Weakly interacting particle systems – de Giorgi formulation

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

$$\dot{\boldsymbol{c}}_{\boldsymbol{x}}(t) = \sum_{\boldsymbol{y}} \left(\boldsymbol{c}_{\boldsymbol{y}}(t)\boldsymbol{Q}_{\boldsymbol{y},\boldsymbol{x}} - \boldsymbol{c}_{\boldsymbol{x}}(t)\boldsymbol{Q}_{\boldsymbol{x},\boldsymbol{y}}\right) = (\boldsymbol{c}(t)\boldsymbol{Q})_{\boldsymbol{x}} = -\left(\mathcal{K}^N(\boldsymbol{c}(t))D\boldsymbol{\mathcal{F}}^N(\boldsymbol{c}(t))\right)_{\boldsymbol{x}}.$$

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

Proposition (Curves of maximal slope)

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

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

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

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A class of nonlinear ODEs

- Gibbs measures $\{\pi(\mu) \in \mathcal{P}(\mathcal{X})\}_{\mu \in \mathcal{P}(\mathcal{X})}$

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

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

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

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

$$\dot{c}_x(t) = \sum_{y \neq x} \left(c_y(t)\, Q_{yx}(c(t)) - c_x(t)\, Q_{xy}(c(t))\right) = \left(c(t)\, Q(c(t))\right)_x$$

- Stationary states π^* are fixed points of

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

Not necessarily unique!

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

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

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

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Formal gradient flow

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

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

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Proposition (Metric)

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

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

where for $\psi \in \mathbf{R}^{\mathcal{X}}$

$$\mathcal{A}(c,\psi) := \langle \psi, \mathcal{K}(c)\psi\rangle_{\mathcal{X}} = \frac{1}{2}\sum_{x,y} w_{xy}(c)\,(\psi_x - \psi_y)^2$$

and (c,ψ) *solves*

$$\dot c(t) = \mathcal{K}(c(t))\psi(t) \qquad \textit{with} \qquad c(0) = \mu \quad \textit{and} \quad c(1) = \nu,$$

is a complete separable metric space.

A class of nonlinear ODEs – de Giorgi formulation

Proposition (Metric)

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

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

where for $\psi \in \mathbf{R}^{\mathcal{X}}$

$$\mathcal{A}(c, \psi) := \langle \psi, \mathcal{K}(c)\psi \rangle_{\mathcal{X}} = \frac{1}{2} \sum_{x,y} w_{xy}(c)\, (\psi_x - \psi_y)^2$$

is a complete separable metric space.

Proposition (Curves of maximal slope)

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

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

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* $t > 0$.

A class of nonlinear ODEs – Liouville equation

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

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- 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

$$\mathbb{W}(\mathbb{M},\mathbb{N}) := \inf_{(\mathbb{C},\Psi)} \int_0^1 \mathbb{A}\left(\mathbb{C}(t),\Psi(t)\right)\, dt \stackrel{!}{=} W_{\mathcal{W}}^2(\mathbb{M},\mathbb{N}) := \inf_{\Pi} \int \mathcal{W}^2(\mu,\nu)\Pi(d\mu,d\nu).$$

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Passage to the limit – Overview and Strategy

Master equation $\boldsymbol{X}_t^N$ Markov $(\mathcal{L}^N, \mathcal{X}^N)$ | $\boldsymbol{c} \in \mathrm{AC}\left([0,t], (\mathcal{P}(\mathcal{X}^N), \boldsymbol{\mathcal{W}}^N)\right)$

$$\dot{\boldsymbol{c}}(t) = -\boldsymbol{\mathcal{K}}^N(\boldsymbol{c}(t)) D\boldsymbol{\mathcal{H}}^N(\boldsymbol{c}(t) \mid \boldsymbol{\pi}) \quad \overset{\text{de Giorgi}}{\Longleftrightarrow} \quad \boldsymbol{\mathcal{J}}^N(\boldsymbol{c}) = 0$$

$$\Downarrow L_\sharp^N \qquad\qquad \Downarrow L_\sharp^N$$

$\mathbb{C}^N$ Markov $(\bar{\mathcal{L}}^N, \mathcal{P}_N(\mathcal{X}))$ | $\mathbb{C}^N \in \mathrm{AC}\left([0,T], (\mathcal{P}(\mathcal{P}_N(\mathcal{X})), \mathbb{W}^N)\right)$

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Liouville equation for ODE on $\mathcal{P}(\mathcal{X})$ | $\mathbb{C} \in \mathrm{AC}\left([0,T], (\mathcal{P}(\mathcal{P}(\mathcal{X})), \mathbb{W})\right)$

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Strategy

Proof Γ-$\liminf$ estimate for $\boldsymbol{J}^N$ wrt. $\mathbb{J}$, whenever $L_\sharp^N \boldsymbol{c} \xrightarrow{d} \mathbb{C}$ on $[0,T]$

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Theorem (Sandier-Serfaty)

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

$$\liminf_{N\to\infty} \frac{1}{N}\boldsymbol{\mathcal{F}}^N(\boldsymbol{c}^N(T)) \geq \mathbb{F}(\mathbb{C}(T)) - \mathcal{F}_0 \quad \textit{with } \mathcal{F}_0 \in \mathbf{R}. \tag{A0}$$

In addition, assume it holds

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

where $(\boldsymbol{c}^N,\boldsymbol{\psi}^N)$ *and* $(\mathbb{C}(t),\Psi(t))$ *are solutions of certain continuity equations.*

$$\liminf_{N\to\infty} \frac{1}{N}\boldsymbol{\mathcal{I}}^N(\boldsymbol{c}^N(t)) \geq \mathbb{I}(\mathbb{C}(t)). \tag{A2}$$

Then, whenever $\boldsymbol{\mathcal{J}}^N(\boldsymbol{c}^N) = 0$ *and* $\boldsymbol{c}^N(0) \xrightarrow{\mathcal{T}} \mathbb{C}(0)$ *such that* $\lim_{N\to\infty}\boldsymbol{\mathcal{F}}^N(\boldsymbol{c}^N(0)) = \mathbb{F}(\mathbb{C}(0)) - \mathcal{F}_0$, *it holds* $\mathbb{J}(\mathbb{C}) = 0$ *and*

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Passage to the limit – Abstract theorem

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Passage to the limit – Verification of assumptions I

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

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

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

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Proof: Decompose relative entropy

$$\frac{1}{N}\mathcal{H}\left(\boldsymbol{\mu}^N \mid \boldsymbol{\pi}^N\right) = \frac{1}{N}\mathcal{H}(\boldsymbol{\mu}^N) + \mathrm{E}_{L_\#^N \boldsymbol{\mu}^N}[U] + \frac{1}{N}\log \boldsymbol{Z}^N$$

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

Passage to the limit – Verification of assumptions I

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Passage to the limit – Verification of assumptions I

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

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

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By Sanov's Theorem:

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

Proposition (Convergence of metric derivative and slopes)

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

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

such that

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

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

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and

$$\liminf_{N\to\infty} \int_0^T \frac{1}{N} \boldsymbol{\mathcal{I}}^N\left(\boldsymbol{c}^N(t)\right) dt \geq \int_0^T \mathbb{I}\left(\mathbb{C}(t)\right) dt. \tag{A2}$$

Passage to the limit – Result

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

$$\frac{1}{N}\boldsymbol{\mathcal{F}}^N(\mathbf{c}^N(0)) \to \mathbb{F}(\mathbb{C}(0)) - \mathcal{F}_0 \qquad \textit{with} \qquad L_\sharp^N \mathbf{c}^N(0) \xrightarrow{d} \mathbb{C}(0) \qquad \textit{as } N \to \infty.$$

Then it holds

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

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

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

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

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

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* κ *is give by*

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κ-convexity – Curie-Weiss model

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

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

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

For the dynamic use for instance Metropolis rates:

$$p_{\mathrm{MC}}(\mu) = \exp\left(-2\beta(\mu(0) - \mu(1))_+\right) \qquad q_{\mathrm{MC}}(\mu) = \exp\left(-2\beta(\mu(1) - \mu(0))_+\right)$$

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- Proof lower bound in $\kappa_{\mathrm{MC}}(\beta) = 2 - 2\beta$
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- Second order approximation of the N-particle system
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