Gradient flow formulation and longtime behaviour of a constrained Fokker-Planck equation

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joint work with Simon Eberle and Barbara Niethammer

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Introduction and Motivation

Fokker-Planck equation: gradient flow and longtime behaviour

Starting point: The classical Fokker-Planck equation

$$\partial_t \rho(t,x) = \partial_x\big(\nu^2 \partial_x \rho(t,x) + H'(x)\rho(t,x)\big)$$

with $\rho(0,x) = \rho^0(x)$ and $\int \rho^0(x)\,\mathrm{d}x = 1$ posses a free energy

$$\mathcal{F}(\rho) = \nu^2 \int \rho(x)\log\rho(x)\;\mathrm{d}x + \int H(x)\rho(x)\,\mathrm{d}x + \mathcal{F}_0.$$

such that it is the gradient flow with respect to the Wasserstein metric

$$\partial_t \rho = -\mathcal{K}(\rho)\,D\mathcal{F}(\rho) \qquad \text{with} \qquad \mathcal{K}(\rho)\varphi := -\partial_x(\rho\,\partial_x\varphi).$$

Convergence to equilibrium via the entropy method:
Set $\gamma_0 := \exp\big(-H/\nu^2\big)/Z_0$ with $Z_0 = \int \exp\big(-H(x)/\nu^2\big)\,\mathrm{d}x$ and $\mathcal{F}_0 = \log Z_0$ then

$$\mathcal{F}(\rho) = \nu^2\mathcal{H}(\rho|\gamma_0) \geq 0 \quad \text{with} = 0 \text{ iff } \rho = \gamma_0.$$

Energy dissipation relation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\rho(t)) = -\int \big|\nu^2\partial_x \log\rho + H'\big|^2\,\mathrm{d}x \leq 0.$$

leads to exponential convergence to equilibrium $\mathcal{F}(\rho(t)) \leq e^{-\frac{t}{C_{\mathrm{LSI}}}}\mathcal{F}(\rho(0))$.

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Fokker-Planck equations: constraint

Motivation:

- Many-particle storage system exposed to external dynamical loading obeying

$$\int x\rho(t,x)\,\mathrm{d}x = \ell(t) \qquad \text{with } \ell \text{ dynamical load.} \qquad \mathcal{C}$$

- Example: Lithium-ion batteries during a charge-discharging cycle[1]

The constraint $\mathcal{C}$ introduces a nonlocal Lagrange multiplier $\sigma(t)$

$$\partial_t \rho(t,x) = \partial_x \left(\nu^2 \partial_x \rho(t,x) + \big(H'(x) - \sigma(t)\big)\,\rho(t,x)\right),$$

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Frst goal: Incorporate constraint in gradient flow formulation[2]

Second goal: Give a characterization of the internal time-scale of relaxation.

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Constrained gradient flow

Constrained gradient flow: Formalism

Constrained state space: $\mathcal{M}^\ell := \{\rho \in \mathcal{P}(\mathbb{R}) : M_1(\rho) = \ell\}$, $M_1(\rho) := \int x\rho(x)\,\mathrm{d}x$.
In general $\mathcal{M}^{\mathcal{C};t} = \{\rho \in \mathcal{P}(\mathbb{R}) : \mathcal{C}(\rho; t) = 0\}$, here $\mathcal{C}(\rho; t) := M_1(\rho) - \ell(t)$.

Assumption: Constraint is nondegenerate

$$\langle D\mathcal{C}(\rho;t), \mathcal{K}(\rho) D\mathcal{C}(\rho;t)\rangle = |\nabla \mathcal{C}(\rho;t)|_\rho^2 > 0.$$

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- Dynamical constraints: augment state space with time dimension
  $\Rightarrow$ pass from nonautonomous system to autonomous

Constrained gradient flow

$\rho : \mathbb{R}_+ \to \mathcal{M}$ is the constrained gradient flow with respect to the nondegenerate dynamical constraint $\mathcal{C} : \mathcal{M} \times \mathbb{R}_+ \to \mathbb{R}$, if for all $t \geq 0$:

$$\partial_t \rho = -\mathcal{K}(\rho(t))D\mathcal{F}(\rho(t)) + \sigma(\rho(t),t)\,\mathcal{K}(\rho(t))D\mathcal{C}(\rho(t),t),$$

$$\text{with} \quad \sigma(\rho,t) = \frac{\langle D\mathcal{F}(\rho), \mathcal{K}(\rho)D\mathcal{C}(\rho,t)\rangle + \partial_t\mathcal{C}(\rho,t)}{|\nabla\mathcal{C}(\rho,t)|_\rho^2}.$$

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Constrained gradient flow: Time-discrete Euler scheme

Let $h > 0$ be a fixed time step and define for $k \geq 1$

$$\rho^k = \operatorname*{arg\,min}_{\rho \in \mathcal{M}^{\ell(kh)}} \left(\frac{1}{2} W_2^2(\rho^{k-1}, \rho) + h\mathcal{F}(\rho) \right).$$

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Assumption: ℓ is Lipschitz and $H \in C^3(\mathbb{R})$ is uniform convex at ∞, that is

$$\lim_{x \to \pm\infty} H''(x) = c_{H,\pm} > 0.$$

Initial data ρ^0 has finite second moment $M_2(\rho^0) < \infty$
and bounded free energy $\mathcal{F}(\rho^0) < \infty$.

Well-posedness: via direct method and convexity of $\mathcal{F}$ and $\mathcal{M}^\ell$

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Passage to the limit $h \to 0$

Let ρ_h be a piecewise constant interpolation of $\{\rho^k\}$ solution of the scheme, then ρ_h converges weakly to a weak solution of the constrained Fokker-Planck equation.

- Time-discrete approximation of the weak formulation: For all $\zeta \in C_c^\infty(\mathbb{R})$

$$\left| \int_{\mathbb{R}} \frac{\rho_h^k - \rho_h^{k-1}}{h} \zeta + \int \left((H'(x) - \sigma_h^k) \partial_x \zeta - \partial_{xx} \zeta \right) \rho^k \right| \leq \sup_{\mathbb{R}} \frac{|\partial_{xx}\zeta|}{2} \frac{1}{h} W_2^2(\rho_h^{k-1}, \rho_h^k),$$

with the discrete Lagrange multiplier σ_h^k given by

$$\sigma_h^k = \int_{\mathbb{R}} H'(x) \rho_h^k(x) \, \mathrm{d}x + \frac{\ell(kh) - \ell((k-1)h)}{h}.$$

- A priori estimates on moments, entropy, energy and Wasserstein distance.
- Uniform convergence of the Lagrange multiplier via an Arzéla-Ascoli argument

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Convergence to equilibrium

Convergence to equilibrium: Problems

Naive application of entropy method fails:

- System is not thermodynamically closed for $\dot{\ell} \neq 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\rho(t)) = -\mathcal{D}(\rho(t),\sigma(t)) + \sigma(t)\,\dot{\ell}(t)$$

with

$$\mathcal{D}(\rho,\sigma) := \int \left|\nu^2\partial_x \log\rho + H' - \sigma\right|^2 \mathrm{d}x = \int \left|\nu^2\partial_x \log\frac{\rho}{\gamma_\sigma}\right|^2 \mathrm{d}x$$

and $\gamma_\sigma(x) = \exp\left(-\frac{H(x)-\sigma x}{\nu^2}\right)/Z_\sigma$.

- Naive use of logarithmic Sobolev inequality does not close the entropy relation, even for $\dot{\ell} \equiv 0$

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(\rho(t)) = -\mathcal{D}(\rho(t),\sigma(t)) \leq -\frac{\nu^2}{C_{\mathrm{LSI}}}\mathcal{H}\big(\rho(t)|\gamma_{\sigma(t)}\big)$$

Mismatch of reference state!

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Idea: Constrained minimization of free energy

Characterization of minimizer

There exists a unique minimizer of the constrained minimization problem

$$\arg\min_{\rho \in \mathcal{M}^\ell} \mathcal{F}(\rho) = \gamma_{\lambda(\ell)} \quad \text{with} \quad \gamma_{\lambda(\ell)}(x) = \frac{1}{Z_{\lambda(\ell)}} \exp\left(-\frac{H(x) - \lambda(\ell)x}{\nu^2} \right)$$

The function $\lambda : \mathbb{R} \to \mathbb{R}$ implicitly defined by $M_1(\gamma_{\lambda(\ell)}) = \ell$ satisfies the Bi-Lipschitz estimate

$$0 < c_{\mathrm{var}} \leq \frac{\mathrm{d}M_1(\gamma_\lambda)}{\mathrm{d}\lambda} \leq C_{\mathrm{var}} < \infty.$$

Proof:

- Convexity of $\mathcal{F}$ and $\mathcal{M}^\ell$ yields uniqueness
- Explicit construction for existence
- Bi-Lipschitz estimate:

$$\frac{\mathrm{d}M_1(\gamma_\lambda)}{\mathrm{d}\lambda} = \int x^2 \gamma_\lambda(x)\,\mathrm{d}x - \left(\int x\, \gamma_\lambda(x)\,\mathrm{d}x \right)^2 =: \mathrm{var}(\gamma_\lambda).$$

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Convergence to equilibrium: Relative entropy and a priori bounds

Relative entropy magic

For all $\eta \in \mathbb{R}$, all $\ell \in \mathbb{R}$ and all $\rho \in \mathcal{M}^\ell$ it holds

$$\frac{c_{\mathrm{var}}}{2}(\eta - \lambda(\ell))^2 \leq \mathcal{H}(\rho|\gamma_\eta) - \mathcal{H}\big(\rho|\gamma_{\lambda(\ell)}\big) \leq \frac{C_{\mathrm{var}}}{2}(\eta - \lambda(\ell))^2$$

- Uniform bounds on moment, Lagrange multiplier and free energy

$$\sup_{t\geq 0} \max\{M_2(\rho(t)), \sigma(t), \mathcal{F}(\rho(t))\} \leq C.$$

- Uniform logarithmic Sobolev estimate

$$\forall |\sigma| \leq C : \qquad \mathcal{H}(\rho|\gamma_\sigma) \leq C_{\mathrm{LSI}} \mathcal{D}(\rho, \sigma).$$

The constant C_{LSI}^{-1} characterizes the rate of convergence to equilibrium

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Convergence to equilibrium

Suppose the dynamical constraint becomes constants

$$\dot{\ell} \in L^1(\mathbb{R}_+) \qquad \Rightarrow \qquad \lim_{t\to\infty} \ell(t) = \ell^*.$$

Then

$$\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) \leq e^{-\frac{t}{C_{\mathrm{LSI}}}} \mathcal{H}\big(\rho^0|\gamma_{\lambda(\ell^0)}\big) + C_{\ell,\sigma} \int_0^t e^{-\frac{t-s}{C_{\mathrm{LSI}}}} |\dot{\ell}(s)| \,\mathrm{d}s.$$

with $C_{\ell,\sigma} = \|\sigma\|_\infty + \|\lambda \circ \ell\|_\infty$.

Proof:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) &= -\mathcal{D}(\rho(t),\sigma(t)) + \dot{\ell}(t)(\sigma(t) - \lambda(\ell(t))) \\ &\leq -\frac{1}{C_{\mathrm{LSI}}}\mathcal{H}\big(\rho(t)|\gamma_{\sigma(t)}\big) + C_{\sigma,\ell}|\dot{\ell}(t)| \\ &\leq -\frac{1}{C_{\mathrm{LSI}}}\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) + C_{\sigma,\ell}|\dot{\ell}(t)|\end{aligned}$$

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$$\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) \leq e^{-\frac{t}{C_{\mathrm{LSI}}}} \mathcal{H}\big(\rho^0|\gamma_{\lambda(\ell^0)}\big) + C_{\ell,\sigma} \int_0^t e^{-\frac{t-s}{C_{\mathrm{LSI}}}} |\dot{\ell}(s)| \,\mathrm{d}s.$$

with $C_{\ell,\sigma} = \|\sigma\|_\infty + \|\lambda \circ \ell\|_\infty$.

Proof:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) &= -\mathcal{D}(\rho(t),\sigma(t)) + \dot{\ell}(t)(\sigma(t) - \lambda(\ell(t))) \\ &\leq -\frac{1}{C_{\mathrm{LSI}}}\mathcal{H}\big(\rho(t)|\gamma_{\sigma(t)}\big) + C_{\sigma,\ell}|\dot{\ell}(t)| \\ &\leq -\frac{1}{C_{\mathrm{LSI}}}\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell(t))}\big) + C_{\sigma,\ell}|\dot{\ell}(t)|\end{aligned}$$

Convergence to equilibrium: Results II

- Fix reference state: For any $\ell^* \in \mathbb{R}$, any $\ell \in \mathbb{R}$ and all $\rho \in \mathcal{M}^\ell$

$$\mathcal{H}(\rho|\gamma_{\lambda(\ell^*)}) \leq \mathcal{H}(\rho|\gamma_{\lambda(\ell)}) + \frac{C_{\mathrm{var}}}{2c_{\mathrm{var}}^2}|\ell^* - \ell|^2.$$

- Let ℓ converge exponentially: $|\dot{\ell}(t)| \leq L_0 e^{-\kappa t}$, then

$$\mathcal{H}\big(\rho(t)|\gamma_{\lambda(\ell^*)}\big) \leq C_0 e^{-\tau\, t} \quad \text{with} \quad \tau = \min\{C_{\mathrm{LSI}}^{-1}, \kappa\}.$$

- Classical Csiszár-Pinsker inequality implies L^1-convergence

$$\int \big|\rho(t,x) - \gamma_{\lambda(\ell^*)(x)}\big| \,\mathrm{d}x \leq \tilde{C}_0 e^{-\frac{\tau}{2}\, t}.$$

- A weighted Csiszár-Pinsker inequality due to [Bolley, Villani 2005] yields

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Thank you for your attention!