1 DDMCS - ATI workshop May 8-10

Position dependent Langevin dynamics

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2 pLD - $\boldsymbol{p}$-dependent noise and friction

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position dependent Langevin dynamics (pLD):

$$\begin{aligned} \frac{d}{dt}\boldsymbol{q} &= \boldsymbol{M}^{-1}\boldsymbol{p} \\ \frac{d}{dt}\boldsymbol{p} &= \boldsymbol{F}(\boldsymbol{q})\mathrm{d}t - \boldsymbol{\Gamma}(\boldsymbol{q})\boldsymbol{p}\mathrm{d}t + \boldsymbol{\Sigma}(\boldsymbol{q})\mathrm{d}\mathbf{B}_t \end{aligned}$$

+ $\boldsymbol{q}$ positions (aka configurations) and $\boldsymbol{p}$ momenta of a finite set of "particles" sharing a d-dimensional domain

+ mass matrix $\boldsymbol{M}$ is symmetric positive definite

+ $\boldsymbol{\Gamma}(\boldsymbol{q})$ is the friction (aka drag, dissipative force)

+ $\boldsymbol{\Sigma}(\boldsymbol{q})\mathrm{d}\mathbf{B}_t$ is the noise (aka random force, temperature)

3 A particular case

$$\frac{d}{dt}\boldsymbol{p} \;=\; -\nabla_{\boldsymbol{q}} U(\boldsymbol{q})\mathrm{d}t - \gamma \boldsymbol{p}\mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}\mathbf{B}_t$$

with

$\gamma > 0$	*constant friction*
β	*the inverse temperature*

⇒ unique invariant distribution with product density:

$\rho_\beta(\boldsymbol{q},\boldsymbol{p}) \;\propto\; e^{-\beta H(\boldsymbol{q},\boldsymbol{p})}$	*Boltzmann distribution*
$H(\boldsymbol{q},\boldsymbol{p}) \;=\; U(\boldsymbol{q}) + \frac{1}{2}\langle \boldsymbol{p}, \boldsymbol{M}^{-1}\boldsymbol{p}\rangle$	*the 'total' energy*

as $\beta^{-1} \to 0$, ρ becomes 'peakier'

⇒ with $\boldsymbol{p}$-dependent friction and noise the form not known; unicity of the steady state, convergence?

4 Results - 1

We show the existence of a unique invariant distribution

+ under natural (sufficient) conditions:

  - $\mathbf{\Gamma}$ positive definite,

  - $\mathbf{\Sigma}$ full rank and uniformly bounded,

  - control on force

+ geometric convergence of observable averages

⇒ proof follows the pattern of Mattingly, Stuart, Higham 2002 who treat the constant case; construct a Lyapunov function; use Harris condition

+ contractivity of (an) embedded chain Hairer, Mattingly 2009

5 Other LD models of interest

+ dissipative particle dynamics (DPD), which is a momentum-conserving, 2nd order, gradient-type system $\Rightarrow$ ask Matthias!

+ Langevin-type systems with velocity dependent coefficients

+ generalized Langevin equation (non-Markovian) Sachs, Leimkuhler, 2018

6 Results - 2, numerical discretization

+ splitting = additive decomposition of the stochastic vector field into components which can be exactly integrated

+ resulting stochastic maps/Markov kernels can be composed to approximate the solution in a single timestep

+ many choices for the sequence of steps; some inherit the ergodicity properties of the SDE system with (slightly) $\neq$ invariant measure

+ efficient numerical procedure based on multiple timestepping relying on a further splitting of the OU equation at each interior timestep $\Rightarrow$ ask Ben!

+ concretely, good numerical methods are needed because we do not know the form of the limit behaviour

I. The main result

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7 Assumptions on friction, noise

$$\frac{d}{dt}\boldsymbol{p} \;=\; \boldsymbol{F}(\boldsymbol{q})\mathrm{d}t - \boldsymbol{\Gamma}(\boldsymbol{q})\boldsymbol{p}\mathrm{d}t + \boldsymbol{\Sigma}(\boldsymbol{q})\mathrm{d}\mathbf{B}_t$$

The spectrum $\sigma(\boldsymbol{\Gamma}(\boldsymbol{q}))$ is such that

$$0 < \inf_{\boldsymbol{q}\in\Omega_q} \min \sigma(\boldsymbol{\Gamma}(\boldsymbol{q})) \leq \sup_{\boldsymbol{q}\in\Omega_q} \max \sigma(\boldsymbol{\Gamma}(\boldsymbol{q})) < +\infty$$

The diffusion matrix has full rank on Ω_q

The spectrum of $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^T$ is such that:

$$\sup_{\boldsymbol{q}\in\Omega_q} \max \sigma(\boldsymbol{\Sigma}(\boldsymbol{q})\boldsymbol{\Sigma}^T(\boldsymbol{q})) < +\infty$$

8 Assumptions on force

There is a potential function U in $\mathcal{C}^2(\Omega_q, \mathbb{R})$ such that:

$$
\begin{aligned}
-\infty &< \inf_{\boldsymbol{q}\in\Omega_q} U(\boldsymbol{q}) \\
\langle \boldsymbol{q}, \boldsymbol{F}(\boldsymbol{q})\rangle &\leq \langle \boldsymbol{q}, -\nabla_{\boldsymbol{q}} U(\boldsymbol{q})\rangle + A \\
\langle \boldsymbol{q}, -\nabla_{\boldsymbol{q}} U(\boldsymbol{q})\rangle &\leq -B\,U(\boldsymbol{q}) - C\langle \boldsymbol{q}, \boldsymbol{q}\rangle + D.
\end{aligned}
$$

for some constants B, $C > 0$ and $A, D \in \mathbb{R}$

$\Rightarrow$ confinement; dominated by gaussian tails

$\Rightarrow$ for $\boldsymbol{F}$ conservative, the above reduces to known asymptotic growth criteria for geometric ergodicity of constant LD on $\Omega_q = \mathbb{R}^n$ (See Mattingly, Stuart, Higham - 2002)

9 The theorem

Suppose force, friction, and noise are as above and all $\mathcal{C}^\infty$

$\Rightarrow$ There is a unique invariant probability μ

$\Rightarrow$ μ has $\mathcal{C}^\infty$ density

$\Rightarrow$ For all $l \in \mathbb{N}$, $\varphi \in L^\infty_{\mathcal{K}_l}$:

$$\|\mathcal{P}_t\varphi - \int_\Omega \varphi \, d\mu\|_{L^\infty_{\mathcal{K}_l}} \leq C_l e^{-\kappa_l t}\|\varphi - \int_\Omega \varphi \, d\mu\|_{L^\infty_{\mathcal{K}_l}}$$

for some constants $\kappa_l, C_l > 0$.

$\Rightarrow$ $L^\infty_{\mathcal{K}_l}$ the Banach space with norm $\sup_\Omega |\phi|/\mathcal{K}_l$ for $\mathcal{K}_l \geq 1$

10 Weights $\mathcal{K}_l \geq 1$

⇒ For $\Omega_q = L\mathbb{T}^n$:

$$\mathcal{K}_l(\boldsymbol{q}, \boldsymbol{p}) = (\langle \boldsymbol{p}, \boldsymbol{p} \rangle + 1)^l,$$

⇒ For $\Omega_q = \mathbb{R}^n$, with suitably chosen constants $a, b, c > 0$:

$$\begin{aligned} \mathcal{K}_l(\boldsymbol{q}, \boldsymbol{p}) &= (aH(\boldsymbol{q}, \boldsymbol{p}) + b\langle \boldsymbol{q}, \boldsymbol{q} \rangle + 2c\langle \boldsymbol{q}, \boldsymbol{p} \rangle)^l \\ H(\boldsymbol{q}, \boldsymbol{p}) &= U(\boldsymbol{q}) + \tfrac{1}{2}\langle \boldsymbol{p}, \boldsymbol{p} \rangle \end{aligned}$$

Also $\mathcal{K}_l \in L_1(\Omega_q \times \mathbb{R}^n, \mu)$

⇒ Follows Mattingly, Stuart, Higham (2002) proof path

II. Example 1 (noise)

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11 Varying temperatures

Temperature depends on the position of the particle

$$\begin{aligned} \mathrm{d}\boldsymbol{q}_i &= \boldsymbol{p}_i \mathrm{d}t \\ \mathrm{d}\boldsymbol{p}_i &= -\nabla_{\boldsymbol{q}_i} U(\boldsymbol{q})\mathrm{d}t - \gamma \boldsymbol{p}_i \mathrm{d}t + \sqrt{2\gamma\left(\beta(\boldsymbol{q}_i)\right)^{-1}}\mathrm{d}\mathbf{B}_t \end{aligned}$$

$\gamma > 0$ is a positive constant, $\beta \in \mathcal{C}^\infty(L\mathbb{T}^d, \mathbb{R}_+)$.

with suitable U the theorem applies

+ the unique invariant measure $\mu_{\gamma,\beta}$ depends nontrivially on γ and β - no closed form!

+ $\Omega_q = \mathbb{R}^n$ one needs to ask for bounded temperatures;

+ periodic simulation box $L\mathbb{T}^d$

12 Temperature gradient

We place $N = 64$ particles on a two dimensional $L\mathbb{T}^2$ ($n = 128$), with a heat source at the center of the simulation box:

$$(\beta(\boldsymbol{q}_i))^{-1} = \Psi\left(\|\boldsymbol{q}_i - c_L\|\right),$$

where $c_L = \frac{1}{2}(L, L)$ is the center of the simulation box, Ψ is a smooth 'bump' function:

$$\begin{aligned}\Psi(r) &= T_{\min} + \Delta T \exp(-\tfrac{1}{1-(r/r_0)^2}) & r \leq r_0 \\ &= T_{\min} & r > r_0\end{aligned}$$

$T_{\min}$, ΔT, r_0 parameters configuring the bump.

13 Force

Pairwise repulsive soft potential:

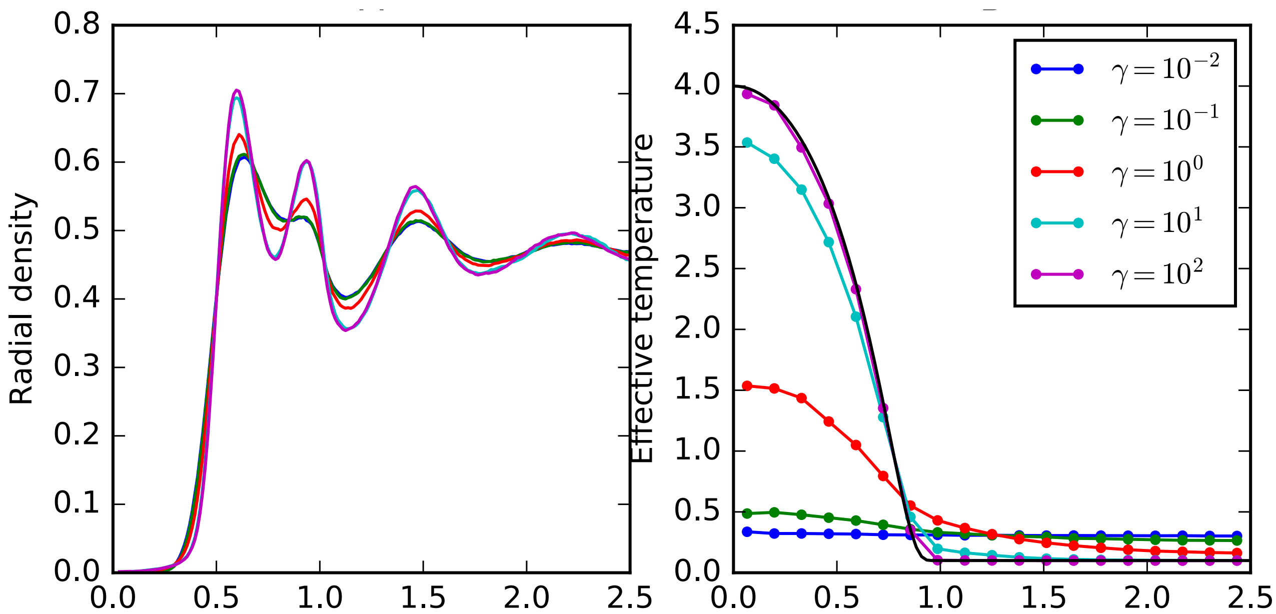
$$\begin{aligned}\omega(r) &= \tfrac{k}{2}(r - c_r)^2 && r < c_r \\ &= 0 && r \geq c_r\end{aligned}$$

with k and c_r positive constants.

+ harmonic potential ('semi-spring')

+ isolated jump discontinuity in the second derivative of the potential

14 radial density and effective temperature

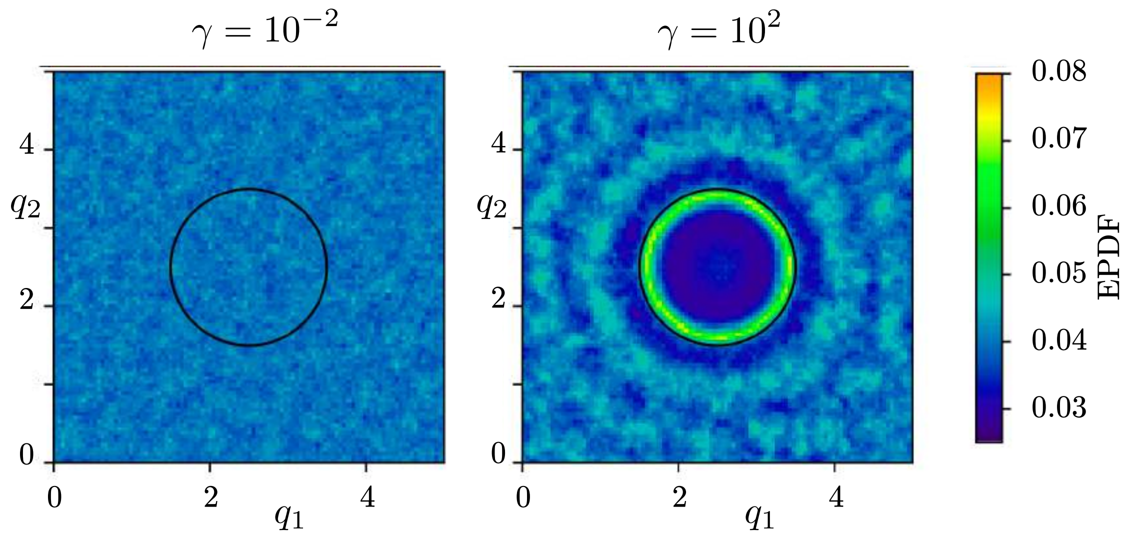


+ radial density function for different values of friction γ
+ distance r from heat source c_L vs. effective temperature:

$$\beta_\gamma^{-1}(r) := \mathbb{E}(\langle \boldsymbol{p}_i, \boldsymbol{p}_i \rangle \mid \|\boldsymbol{q}_i - c_L\| = r)$$

+ black curve corresponds to the temperature $\Psi(r)$

15 Particle density



Empirical particle density calculated as a cumulative average over the simulation time, for low and high friction

The area inside the black circle corresponds to the heat source bump.

III. Example 2 (non-conservative force)

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16 System with non-conservative force

$\Omega_q = \mathbb{R}^n$ with $n = 2$ and let the force $\mathbf{F}$ be of the form:

$$\begin{aligned} \boldsymbol{F}(\boldsymbol{q}) &= -\nabla_{\boldsymbol{q}} U(\boldsymbol{q}) + \alpha\, \boldsymbol{J}\, \boldsymbol{q}, \\ U(\boldsymbol{q}) &= \textstyle\sum_{i=1}^{2} (\boldsymbol{q}_i^2 - 1)^2, \end{aligned}$$

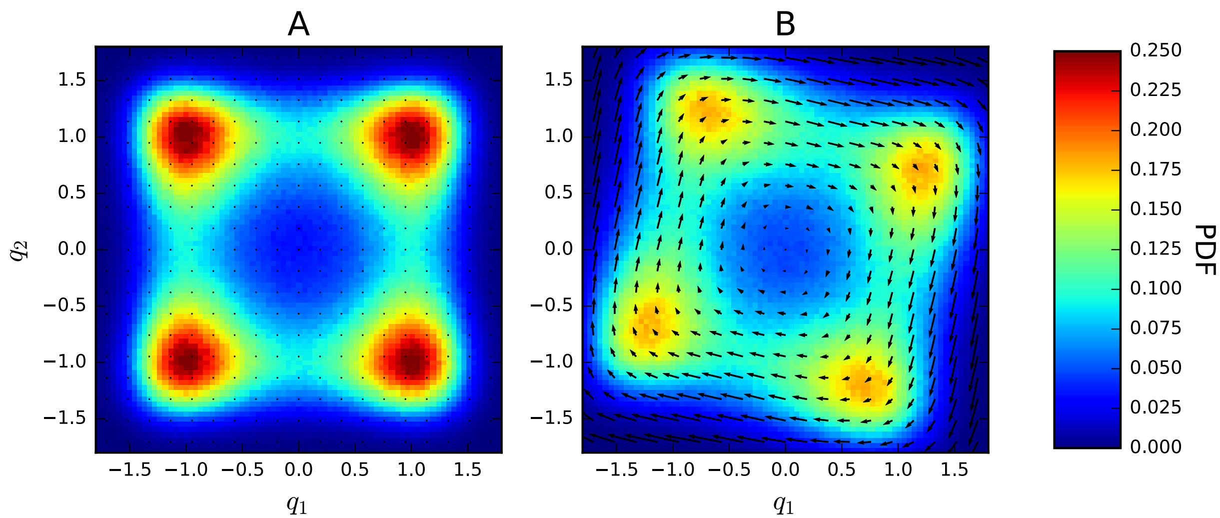
with the antisymmetric:

$$\boldsymbol{J} := \frac{3}{2} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

For $\alpha = 0$, the system resembles a particle moving in a 4-well potential driven by standard LD; with minima of U at $(\pm 1, \pm 1)$ and Boltzmannian invariant density

The non-conservative force $\alpha\, \boldsymbol{J}\, \boldsymbol{q}$, corresponds to a stirring force, which pushes the system clockwise direction around the origin.

17 Positional density



$\boldsymbol{q}$ marginals of the invariant density: $\alpha = 0$: Boltzmannian invariant density; $\alpha = 1$: rotated and smeared invariant density

arrows correspond to estimates of the mean momentum in the invariant density; we see a vector field spiralling clockwise around the origin

IV. Example 3: (friction)

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18 modified stochastic Cucker-Smale

Blended Langevin model for flocking à la Cucker-Smale $\rightarrow$ see Entropy paper

19 Idea of a sorting model (phase separation)

Consider a general xLD with typed particles:

$$\begin{aligned} \dot{q}_i &= p_i \\ \dot{p}_i &= -\nabla U(q_i) - \Gamma_i(q_i)p_i + \Sigma_i dB_t \end{aligned}$$

We write ϵ_i for type of particle i.

We set the friction term as follows:

$$\Gamma_i(q_i) \;=\; \textstyle\sum_{j\in\mathcal{N}(q_i)} \gamma_{\epsilon_i\epsilon_j}$$

where $\mathcal{N}(q_i^\epsilon)$ is the Euclidean ball of radius r centered at q_i (which includes the particle i itself), $\gamma_{\epsilon\epsilon'}$ is the adhesion 'tensor'.

Suppose off-diagonal terms $\gamma_{\epsilon\epsilon'}$ in the adhesion tensor are smaller than diagonal ones $\rightarrow$ phase separation? (which could also be modelled by type-dependent repulsion).

could change the type of particle j on the fly for opinion formation!

20 Qs

+ develop biological tissue examples (phase separation)

+ Q - can we infer friction and noise?

+ specifically using IRL techniques from 'Inverse Reinforcement Learning in Swarm Systems' for particle systems?

+ constructive versions?

+ limited to domains with no boundaries