Particle systems with singular interaction for Wasserstein-type diffusion

Vitalii Konarovskyi

Bielefeld University

Mathphys Analysis Seminar – ISTA

joint work with Max von Renesse

UNIVERSITÄT BIELEFELD

National Academy of Sciences of Ukraine
INSTITUTE OF MATHEMATICS

Table of Contents

Finite Interacting Particle System

Consider interacting particle system

$$dX_t^i = -\frac{1}{n}\sum_{j=1}^{n} \nabla V(X_t^i - X_t^j)dt + \sqrt{n}dw_t^i, \quad i = 1, \dots, n,$$

where w^i are independent Brownian motions.

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where w^i are independent Brownian motions.
Assume that the mass of every particle equals $\frac{1}{n}$ the evolution of particle mass

$$\mu_t = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_t^i}, \quad t \geq 0,$$

is described by the **Dean-Kawasaki equation**

$$\frac{\partial}{\partial t}\mu_t = \frac{n}{2}\Delta\mu_t + \nabla\cdot(\mu_t \nabla V * \mu_t) + \nabla\cdot\left(\sqrt{\mu_t}\dot{W}_t\right)$$

[Kawasaki (Physica A '94), Dean (J Phys A '96)]

Dean-Kawasaki Equation

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The equation is used for modeling of evolution of particle mass in the Langevin dynamics.

[K. Kawasaki '94; D. Dean '96; A. Donev, E. Vanden-Eijnden '14, '15, '22; B. Derrida '16; F. Cornalba, J. Zimmer '19, '20, '21; B. Gess '19, F. Cornalba, J. Fischer '21, F. Cornalba, J. Fischer, J. Ingmanns '23 . . .]

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Definition of Solution

A continuous process μ_t, $t \geq 0$, is a solution to the D-K equation if $\forall\varphi \in \mathcal{C}_b^2(\mathbb{R}^d)$

$$\langle\varphi, \mu_t\rangle - \langle\varphi, \mu_0\rangle - \frac{\alpha}{2}\int_0^t \langle\Delta\varphi, \mu_s\rangle ds + \int_0^t \langle\nabla\varphi\cdot(\nabla V * \mu_s), \mu_s\rangle\, ds$$

is a martingale with quadratic variation $\int_0^t \langle|\nabla\varphi|^2, \mu_s\rangle ds$.

Well-Posedness of Dean-Kawasaki Equation

The empirical process

$$\mu_t = \frac{1}{n}\sum_{i=1}^{n} \delta_{X_t^i}, \quad t \geq 0,$$

where

$$dX_t^i = -\frac{1}{n}\sum_{j=1}^{n} \nabla V(X_t^i - X_t^j)dt + \sqrt{n}dw_t^i, \quad i = 1, \dots, n,$$

is a solution to the DK equation for $\alpha = n \in \mathbb{N}$ started from $\mu_0 = \sum_{i=1}^{n} \delta_{X_0^i}$.

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Theorem [K., Lehmann, von Renesse, ECP '19, J. Stat. Phys. '20]

Let $\mu_0(\mathbb{R}^d) = 1$ and $V \in \mathcal{C}_b^2(\mathbb{R}^d)$. Then the DK equation has a (unique) solution if and only if $\alpha = n$ and $\mu_0 = \frac{1}{n}\sum_{i=1}^{n} \delta_{x^i}$.

Main Goal

The correction of the equation is needed.

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1. Regularization of noise
   [Cornalba, Shardlow, Zimmer (SIAM JMA, Nonlinearity '20, J. Diff. Eq. '21); Fehrman, Gess '21]

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We want to construct a non-trivial particle model whose mass evolution is described by SPDE

$$\frac{\partial}{\partial t}\mu_t = \Gamma(\mu_t) + \nabla \cdot \left(\sqrt{\mu_t}\dot{W}_t\right)$$

for some (probably singular) Γ.

Table of Contents

Rimannian structure on Wasserstein space

Wasserstein Metric on $\mathcal{P}_2(\mathbb{R}^d)$ and **Benamou-Brenier formula**:

$$\mathcal{W}_2^2(\rho^1,\rho^2) := \inf\left\{\mathbb{E}|\xi^1-\xi^2|^2 : \ \xi^i \sim \rho^i\right\}$$

$$= \inf\left\{\int_0^1\int_{\mathbb{R}^n}|\nabla\Phi(t,x)|^2\rho(t,x)dxdt : \begin{array}{r}\partial_t\rho(t,x)+\nabla\cdot(\rho(t,x)\nabla\Phi(t,x))=0,\\ \rho(0,x)=\rho^1,\ \rho(1,x)=\rho^2(x)\end{array}\right\}$$

$$= \inf\left\{\int_0^1 g_{\rho_t}(\dot\rho_t,\dot\rho_t)dt : \ \rho_0=\rho^1,\ \rho_1=\rho^2, \quad \dot\rho_t\in T_{\rho_t}\mathcal{P}_2\right\}$$

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Wasserstein Gradient:

$$\mathrm{grad}_{\mathcal{W}} F(\rho) = -\nabla\cdot\left(\rho\nabla\frac{\delta}{\delta\rho}F(\rho)\right).$$

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$\rightsquigarrow$ Heat equation

$$\frac{\partial\mu_t}{\partial t} = \frac{\alpha}{2}\Delta\mu_t$$

is a gradient flow on the Wasserstein space:

$$\frac{\partial\mu_t}{\partial t} = -\operatorname{grad}_{\mathcal{W}}\left[\frac{\alpha}{2}E(\mu_t)\right] \qquad \text{[Otto (CPDE'01)]}$$

where $E(\rho) = \int_{\mathbb{R}^d}\rho(x)\ln\rho(x)dx$

Dean-Kawasaki equation and Wasserstein Geometry

Heat equation

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is a gradient flow on the Wasserstein space:

$$\frac{\partial \mu_t}{\partial t} = -\operatorname{grad}_{\mathcal{W}} [\alpha E(\mu_t) + F(\mu_t)] + \dot{B}_t,$$

where

- $E(\rho) = \int_{\mathbb{R}^d} \rho(x) \ln \rho(x) dx$;

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- $E(\rho) = \int_{\mathbb{R}^d} \rho(x) \ln \rho(x) dx$;
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- $F(\mu) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} V(x-y)\mu(dx)\mu(dy)$;
- B_t is a “Brownian motion” on $\mathcal{P}_2$ since the quadratic variation of $G(\mu_t)$ is given by

$$\int_0^t \left\langle \left| \nabla \frac{\partial G(\mu_s)}{\partial \mu_s} \right|^2, \mu_s \right\rangle ds = \int_0^t g_{\mu_s}\left(\operatorname{grad}_{\mathcal{W}} G(\mu_s), \operatorname{grad}_{\mathcal{W}} G(\mu_s)\right) ds.$$

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$\rightsquigarrow$ μ_t **can be interpreted as a Brownian motion (with drift) on** $\mathcal{P}_2$

Short-time asymptotic of a Brownian motion

Short-time asymptotic formula for a heat kernel

$$p(t,x,y) = \frac{1}{(2\pi t)^{n/2}} e^{-\frac{\|x-y\|^2}{2t}} \sim e^{-\frac{\|x-y\|^2}{2t}}, \quad t \to 0+.$$

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Generalizations

- Heat equation with variable coefficients in $\mathbb{R}^n$ [Varadhan (CPAM '67)]
- Smooth Riemannian manifold with Ricci curvature bound [P. Li and S.-T. Yau (Acta Math. '86)]
- Lipschitz Riemannian manifold without any sort of curvature bounds [J. Norris (Acta Math. 97)]
- Infinite-dimensional case for heat kernel generated by a Dirichlet form [J. Ramírez (CPAM '01, Ann. Prob '03)]

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Corollary

If B_t, $t \geq 0$, is a Brownian motion on a Riemannian manifold, then

$$\mathbb{P}_x \{B_t = y\} \sim e^{-\frac{d^2(x,y)}{2t}}, \quad t \to 0+,$$

with d being the Riemannian distance.

Main Goal

We want to construct a non-trivial particle model whose mass evolution is described by SPDE

$$\frac{\partial}{\partial t}\mu_t = \Gamma(\mu_t) + \nabla \cdot \left(\sqrt{\mu_t}\dot{W}_t\right)$$

for some (probably singular) Γ for which **Varadhan's formula**

$$\mathbb{P}\{\mu_t = \nu\} \sim e^{-\frac{\mathcal{W}_2^2(\mu_0,\nu)}{2t}}, \quad t \to 0+,$$

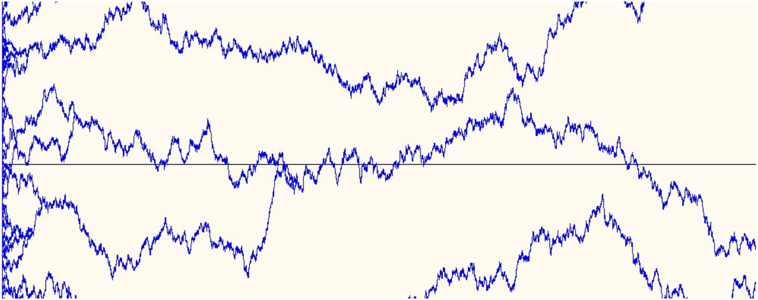
holds with **Wasserstein distance** $\mathcal{W}_2$.

Table of Contents

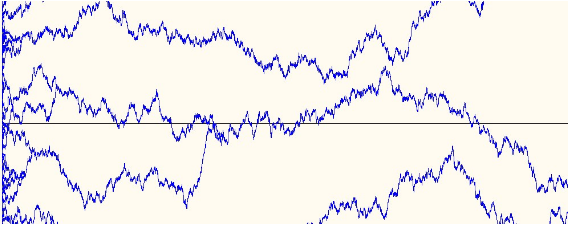
Coalescing particle system: Arratia flow

Arratia flow on $\mathbb{R}$ [R. Arratia '79]

- Brownian particles start from every point of an interval;
- they move independently and coalesce after meeting;



Mathematical description of Arratia flow



$X(u,t)$ is the position of particle at time t starting at u

1. $X(u,0) = u$;
2. $X(u,\cdot)$ is a Brownian motion in $\mathbb{R}$;
3. $X(u,t) \le X(v,t)$, $u < v$
4. $\langle X(u,\cdot), X(v,\cdot)\rangle_t = \int_0^t \mathbb{I}_{\{X(u,s)=X(v,s)\}} ds$.

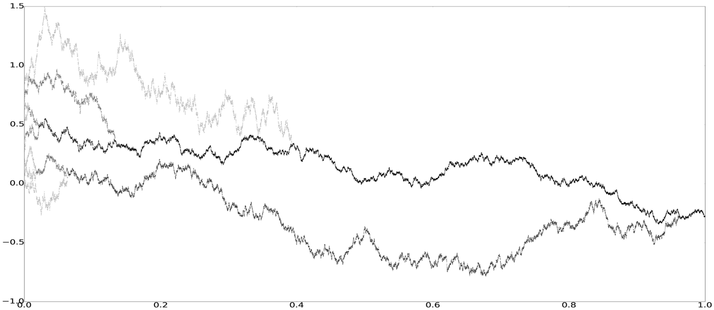
Arratia flow and its generalization

- **Arratia flow appears as scaling limit of different models**
  - true self-repelling motion [B.Tóth and W. Werner (PTRF '98)]
  - isotropic stochastic flows of homeomorphisms in $\mathbb{R}$ [V. Piterbarg (Ann. Prob. '98)]
  - Hastings-Levitov planer aggregation models [J. Norris, A. Turner (Comm. Math. Phys. '12)], etc. . .
- **Further investigation of the Arratia flow**
  - Properties of generated σ-algebra [B. Tsirelson (Probab. Surv. '04)]
  - n-particle motion [R. Tribe, O.V. Zaboronski (EJP '04, Comm. Math. Phys. '06)]
  - large deviations [A. Dorogovtsev, O. Ostapenko (Stoch. Dyn. '10)], etc. . .
- **Generalizations**
  - Brownian web [C. M. Newman et al. (Ann. Prob. '04), R. Sun, J.M Swart (MAMS, '14)]
  - Coalescing non-Brownian particles [S. Evans et al. (PTRF, '13)]
  - Stochastic flows of kernels [Y. Le Jan and O. Raimond (Ann. Prob. '04)]

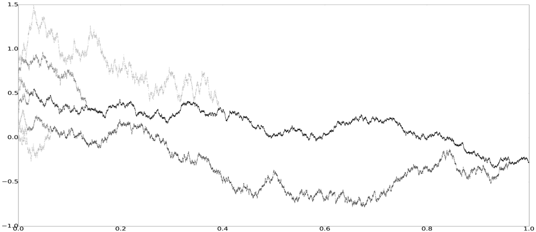
Modified Massive Arratia flow

Modified massive Arratia flow on $\mathbb{R}$ [K. (Ann. Prob. '17, EJP '17)]

- Brownian particles start from points with masses;
- they move independently and coalesce after meeting;
- particles sum their masses after meeting and diffusion rate is inversely proportional to the mass.



Mathematical description



$Y(u,t)$ is the position of particle at time t labeled by $u \in (0,1)$

1. $Y(u,0) = u$;
2. $Y(u,\cdot)$ is a continuous martingale;
3. $Y(u,t) \leq Y(v,t)$, $u < v$;
4. $\langle Y(u,\cdot), Y(v,\cdot)\rangle_t = \int_0^t \frac{\mathbb{I}_{\{Y(u,s)=Y(v,s)\}}}{m(u,s)} ds$.

Measure-valued diffusion and Dean-Kawasaki equation

Theorem [K., Renesse, CPAM '19]

The process $\mu_t = Y(\cdot, t)\big|_{\#} \mathrm{Leb}_{[0,1]}$, $t \geq 0$, that describes the evolution of particle masses in the modified massive Arratia flow solves the equation

$$d\mu_t = \frac{1}{2}\Delta\mu_t^* dt + \nabla \cdot (\sqrt{\mu_t} dW_t),$$

with $\mu_t^* = \sum_{x \in \mathrm{supp}\, \mu_t} \delta_x$ and a white noise dW_t. It also satisfies Varadhan's formulat

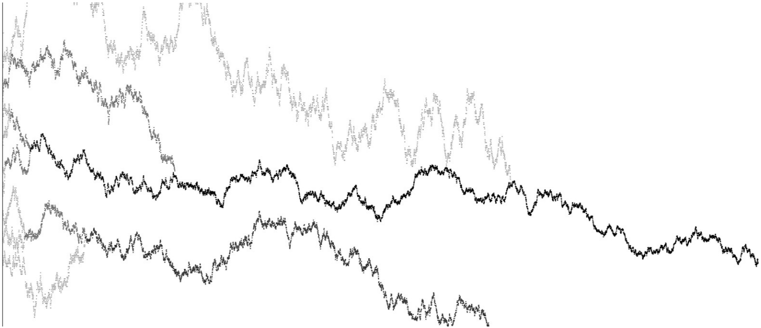
$$\mathbb{P}\{\mu_t = \nu\} \sim e^{-\frac{\mathcal{W}_2^2(\mathrm{Leb}_{[0,1]}, \nu)}{2t}}, \quad t \to 0+,$$

with the Wasserstein distance $\mathcal{W}_2$ in $\mathcal{P}_2(\mathbb{R})$.

Table of Contents

Splitting of Particles

Can we replace coalescing by another type of interaction that would lead to a reversible model?



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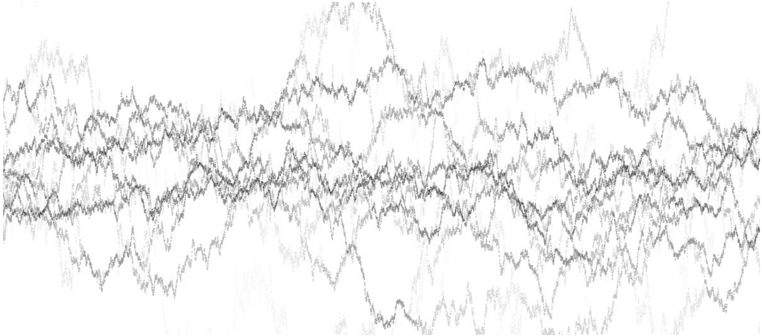

Sticky-Reflected Particle System

Recall that the modified massive Arratia flow Y satisfies

1. $Y(u,0) = u,\ u \in [0,1]$
2. $Y(u,\cdot)$ – continuous martingale
3. $Y(u,t) \leq Y(v,t),\ u < v;$
4. $\langle Y(u,\cdot), Y(v,\cdot)\rangle_t = \int_0^t \frac{\mathbb{I}_{\{Y(u,s)=Y(v,s)\}}}{m(u,s)} ds,\ m(u,s) = \mathrm{Leb}\{w : Y(w,t) = Y(u,t)\}.$

$Y(u,t)$ is particle position at time t started from u

Sticky-Reflected Particle System

Recall that the modified massive Arratia flow Y satisfies

1. $Y(u,0) = g(u)$, $u \in [0,1]$, where $g \uparrow$;
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3. $Y(u,t) \leq Y(v,t)$, $u < v$;
4. $\langle Y(u,\cdot), Y(v,\cdot)\rangle_t = \int_0^t \frac{\mathbb{I}_{\{Y(u,s)=Y(v,s)\}}}{m(u,s)} ds$, $m(u,s) = \mathrm{Leb}\{w : Y(w,t) = Y(u,t)\}$.

$Y(u,t)$ is particle position at time t started from $g(u)$
(the initial mass distribution $= \mathrm{Leb} \circ g^{-1}$).

Sticky-Reflected Particle System

Recall that the modified massive Arratia flow Y satisfies

1. $Y(u,0) = g(u)$, $u \in [0,1]$, where $g \uparrow$;
2. $Y(u,\cdot) - \int_0^t \left(\xi(u) - \frac{1}{m(u,s)} \int_{\pi(u,s)} \xi(r)dr\right) ds$ – continuous martingale, where $\pi(u,t) = \{v : \ Y(u,t) = Y(v,t)\}$ and $\xi \uparrow$ – **interaction potential;**
3. $Y(u,t) \leq Y(v,t)$, $u < v$;
4. $\langle Y(u,\cdot), Y(v,\cdot)\rangle_t = \int_0^t \frac{\mathbb{I}_{\{Y(u,s)=Y(v,s)\}}}{m(u,s)} ds$, $m(u,s) = \mathrm{Leb}\{w : Y(w,t) = Y(u,t)\}$.

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Role of Interaction Potential ξ

Remark that $Y(u,\cdot) - \int_0^t \left(\xi(u) - \frac{1}{m(u,s)} \int_{\pi(u,s)} \xi(r)dr\right) ds$ is a continuous martingale, where $\pi(u,t) = \{v : \ Y(u,t) = Y(v,t)\}$ and $\xi \uparrow$.

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- If ξ is a constant on $\pi(u,t)$, then particle u does not have any drift at t.

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- If $\xi = 0$, then particles coalesce.
- If ξ is a constant on $\pi(u,t)$, then particle u does not have any drift at t.
- If $\xi(u) = \xi(v)$, then particles u and v coalesce after meeting:
  because the drifts $Y(u,\cdot)$ and $Y(v,\cdot)$ at time s equal each other after the meeting

$$\xi(u) - \frac{1}{m(u,s)} \int_{\pi(u,s)} \xi(u)du = \xi(v) - \frac{1}{m(v,s)} \int_{\pi(v,s)} \xi(r)dr,$$

  due to $\pi(u,s) = \pi(v,s)$ for $Y(u,s) = Y(v,s)$.

Role of Interaction Potential ξ

Remark that $Y(u,\cdot) - \int_0^t \left(\xi(u) - \frac{1}{m(u,s)}\int_{\pi(u,s)} \xi(r)dr\right) ds$ is a continuous martingale, where $\pi(u,t) = \{v : \ Y(u,t) = Y(v,t)\}$ and $\xi \uparrow$.

- If $\xi = 0$, then particles coalesce.
- If ξ is a constant on $\pi(u,t)$, then particle u does not have any drift at t.
- If $\xi(u) = \xi(v)$, then particles u and v coalesce after meeting:
  because the drifts $Y(u,\cdot)$ and $Y(v,\cdot)$ at time s equal each other after the meeting

$$\xi(u) - \frac{1}{m(u,s)} \int_{\pi(u,s)} \xi(u)du = \xi(v) - \frac{1}{m(v,s)} \int_{\pi(v,s)} \xi(r)dr,$$

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$\rightsquigarrow$ Since $g(u)=g(v)$, $\xi(u)=\xi(v)$, then $Y(u,\cdot)=Y(v,\cdot)$.

$\rightsquigarrow$ If $g=\sum_{i=1}^n x_i\mathbb{I}_{\pi_i}$, $\xi=\sum_{i=1}^n \xi_i\mathbb{I}_{\pi_i}$, then

$$Y(u,t)=\sum_{i=1}^n x_i(t)\mathbb{I}_{\pi_i}(u).$$

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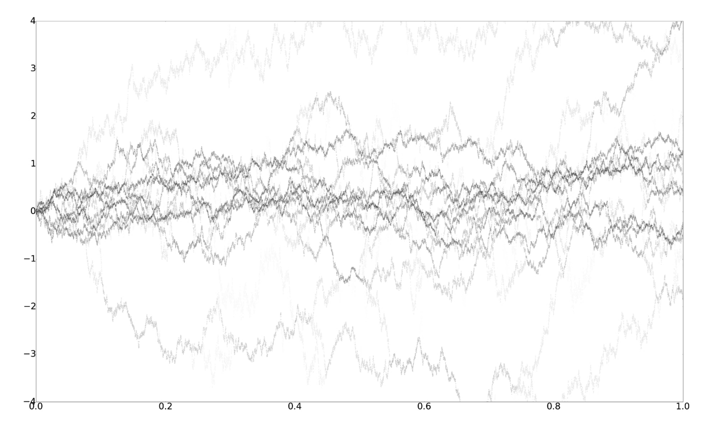

$$g(u) = 0, \quad \xi(u) = u, \quad u \in (0,1)$$

The model is similar to the Howitt-Warren flow, where particles do not change their diffusion rate. [Howitt, Warren (Ann. Probab. '09); Schertzer, Sun, Swart (Mem. Amer. Math. Soc. '14)]

Existence of Particle System

Theorem [K. (Ann. Inst. H. Poincaré, '23)]

Let $g, \xi : [0,1] \to \mathbb{R}$ be nondecreasing and $\frac{1}{2}+$-Hölder continuous. Then there exists a family of continuous processes $Y(u,\cdot)$, $u \in [0,1]$, such that

1. $Y(u,0) = g(u)$
2. $Y(u,\cdot) - \int_0^t \left(\xi(u) - \frac{1}{m(u,s)} \int_{\pi(u,s)} \xi(r) dr \right) ds$ – is a martingale, where $\pi(u,t) = \{v : \ Y(u,t) = Y(v,t)\}$, $m(u,s) = \mathrm{Leb}\{w : Y(w,t) = Y(u,t)\}$;
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Uniqueness of distribution is still an important open problem.

Number of Particles

Let $N(t)$ be a number of distinct particles at time t.

Theorem [K. (TSP, '20)]

1. $\int_0^t \mathbb{E}N(t)dt < \infty$ a.s.

Number of Particles

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Theorem **[K. (TSP, '20)]**

1. $\int_0^t \mathbb{E}N(t)dt < \infty$ a.s.
2. If ξ takes infinitely many values. Then

$$\mathbb{P}\{\exists \text{ a dense set } R \subset [0,\infty) : \quad N(t) = +\infty \quad \forall t \in R\} = 1$$

SDE in $L_2^{\uparrow}$ for Particle System

There exists a white noise such that

$$dY(u,t) = \frac{1}{m(u,t)} \int_{\pi(u,t)} W(dr,dt) + \left(\xi(u) - \frac{1}{m(u,t)} \int_{\pi(u,t)} \xi(r) dr \right) dt.$$

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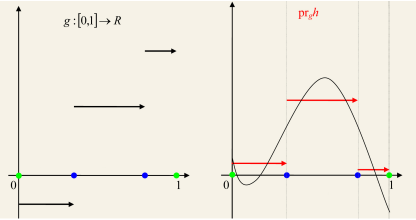
Where pr_g is **the projection** in $L_2[0,1]$ to

$$L_2(g) = \{f : f \quad - \quad \sigma(g)\text{-measurable}\}$$



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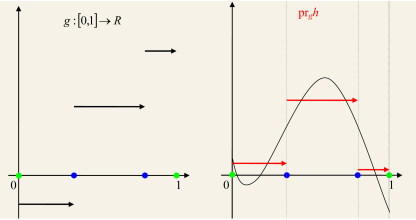

Then $Y_t := Y(\cdot, t) \in L_2^{\uparrow}$ solves the SDE

$$dY_t = \mathrm{pr}_{Y_t} dW_t + (\xi - \mathrm{pr}_{Y_t} \xi)dt.$$

Invariant Measure for Particle System

Define a σ-finite measure $L_2^{\uparrow}$ as follows

$$\Xi = \sum_{n=1}^{\infty} \Xi^n,$$

where

$$\Xi^n \quad \text{is the distribution of} \quad \sum_{k=1}^{n} \mathbb{I}_{[q_{k-1}, q_k)} x_k$$

with jump points $0 = q_0 < q_1 < \cdots < q_{n-1} < q_n = 1$ are distributed according to

$$d\nu_\xi^n = \prod_{k=1}^{n} (q_k - q_{k-1}) d\xi(q_1) \ldots \xi(q_{n-1})$$

and the values of jumps $x_1 \leq \cdots \leq x_n$ are distributed according to $\mathrm{Leb}_{x_1 \leq \cdots \leq x_n}$.

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One can see that $\operatorname{supp} \Xi = L_2^{\uparrow}(\xi) = \{f \in L_2^{\uparrow} : \ f \ - \ \sigma(\xi)\text{-measurable}\}$

Reversible Particle System

Theorem **[K., Renesse '17]**

For any non-decreasing right-continuous function ξ there exists a Markov process Y in $L_2^{\uparrow}(\xi)$ such that

- Ξ – in an invariant measure for Y.
- Y_t is a solution to

$$dY_t = \mathrm{pr}_{Y_t} dW_t + (\xi - \mathrm{pr}_{Y_t} \xi)dt \quad \text{in } L_2^{\uparrow}[0,1].$$

- The evolution of particle mass $\mu_t = \mathrm{Leb} \circ Y^{-1}(\cdot, t)$, solves the equation

$$\frac{\partial}{\partial t}\mu_t = \frac{1}{2}\Delta\mu_t^* + \nabla \cdot (\sqrt{\mu_t}\dot{W}_t), \quad \text{in } \mathcal{P}_2(\mathbb{R}),$$

with $\mu_t^* = \sum_{x \in \mathrm{supp}\, \mu_t} \delta_x$.

- $\mathbb{P}\{\mu_t = \nu\} \sim e^{-\frac{\mathcal{W}_2(\mu_0,\nu)}{2t}}, \quad t \to +0.$

Dirichlet Form Approach

- **Invariant measure:**

$$\Xi = \sum_{n=1}^{\infty} \Xi^n,$$

where Ξ^n: $n-1$ jumps are distributed according

$$d\nu_\xi^n = \prod_{k=1}^{n} (q_k - q_{k-1}) d\xi(q_1) \dots \xi(q_{n-1}),$$

n-values are distributed according to $\mathrm{Leb}_{x_1 \leq \dots \leq x_n}$

- **Space of "smooth" functions:**

$$\mathcal{FC} = \left\{ U = u(\langle h_1, \cdot \rangle_{L_2}, \dots, \langle h_k, \cdot \rangle_{L_2}) \varphi(\| \cdot \|_{L_2}^2) \right\};$$

- **Differential operator:** $\mathrm{D}U(g) = \mathrm{pr}_g \nabla^{L_2} U(g) \in L_2[0,1]$;

(Ex. $\mathrm{D}u(\langle h, g \rangle_{L_2}) = u'(\langle h, g \rangle_{L_2}) \, \mathrm{pr}_g \, h, \quad \mathrm{D}\|g\|_{L_2}^2 = 2g$)

Integration by parts and Dirichlet form

Integration by parts [K., von Renesse '17]

Let $U, V \in \mathcal{FC}$. Then

$$\int_{L_2^\uparrow} (\mathrm{D}U(g), \mathrm{D}V(g))\Xi(dg) = -\int_{L_2^\uparrow} LU(g)V(g)\Xi(dg) - \int_{L_2^\uparrow} V(g)(\nabla^{L_2} U(g), \xi - \mathrm{pr}_g\, \xi)\Xi(dg).$$

(Ex. $Lu((h,g)) = u''((h,g))\|\mathrm{pr}_g\, h\|_{L_2}^2, \quad L\|g\|_{L_2}^2 = 2\#g$)

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(Ex. $Lu((h,g)) = u''((h,g))\|\mathrm{pr}_g\,h\|_{L_2}^2, \quad L\|g\|_{L_2}^2 = 2\#g$)

Dirichlet form:

$$\mathcal{E}(U,V) = \frac{1}{2}\int_{L_2^{\uparrow}(\xi)} (\mathrm{D}U(g), \mathrm{D}V(g))\Xi(dg), \quad U, V \in \mathcal{FC}$$

Theorem [K., von Renesse '17]

$\mathcal{E}$ is a closable bilinear form on $L_2(L_2^{\uparrow}, \Xi)$, its closure is a quasi-regular local symmetric Dirichlet form and $\|\cdot\|_{L_2}$ is its intrinsic metric.

Comparison with Existing Wasserstein-type Models

$$\frac{\partial}{\partial t}\mu_t = \Gamma(\mu_t) + \nabla \cdot \left(\sqrt{\mu_t}\dot{W}_t\right)$$

- **Coalescing-Fragmentating Wasserstein Diffusion**:
  - particles on $\mathbb{R}$;
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- **Dirichlet-Ferguson Diffusion** [Dello Schiavo (Ann. Prob. '22)]:
  - particles on d-dim closed Riemannian manifold, $d \geq 2$;
  - invariant measure – Dirichlet-Ferguson distribution;
  - no interaction.

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