Conservative SPDEs as Fluctuating Mean Field Limits of Stochastic Gradient Descent

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SFB-Kolloquium — Potsdam

joint work with Benjamin Gess and Rishabh Gvalani





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Supervised Learning

• Having a large sets of data $\{(\theta_i, \gamma_i), i \in I\}$, $\theta_i \sim \vartheta$ i.i.d., one needs to find a function $f : \Theta \to \mathbb{R}$ such that $f(\theta_i) = \gamma_i$.

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- Usually one approximates f by

$$f_n(\theta;x) = \frac{1}{n} \sum_{k=1}^n \Phi(\theta,x_k),$$

where $x_k \in \mathbb{R}^d$, $k \in \{1, ..., n\}$, are parameters which have to be found.

Example:
$$\Phi(\theta, x_k) = c_k \cdot h(A_k \theta + b_k), \quad x_k = (A_k, b_k, c_k)$$

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• We measure the distance between f and f_n by the **generalization error**

$$\mathcal{L}(x) := \frac{1}{2} \mathbb{E}_{\vartheta} |f(\theta) - f_n(\theta; x)|^2 = \frac{1}{2} \int_{\Theta} |f(\theta) - f_n(\theta; x)|^2 \vartheta(d\theta),$$

where ϑ is the distribution of θ_i .



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The parameters x_k , $k \in \{1, \ldots, n\}$ can be learned by stochastic gradient descent

$$x_k(t_{i+1}) = x_k(t_i) - \nabla_{x_k} \left(\frac{1}{2}|f(\theta_i) - f_n(\theta_i;x)|^2\right) \Delta t$$

where Δt – learning rate, $t_i = i\Delta t$, $\theta_i \sim \vartheta$ – i.i.d.,

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= $x_k(t_i) - (f_n(\theta_i; x) - f(\theta_i)) \nabla_{x_k} \Phi(\theta_i, x_k(t_i)) \Delta t$

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where Δt – learning rate, $t_i = i\Delta t$, $\theta_i \sim \vartheta$ – i.i.d., $F(x,\theta) = f(\theta)\Phi(\theta,x)$ and $K(x,y,\theta) = \Phi(\theta,x)\Phi(\theta,y)$.

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Continuous Dynamics of Parameters

Recall that $x_k(0) \sim \mu_0$ – i.i.d., Δt – learning rate, $t_i = i\Delta t$, $\theta_i \sim \vartheta$ – i.i.d.

$$x_k(t_{i+1}) = x_k(t_i) + V(x_k(t_i), \nu_{t_i}^n, \theta_i) \Delta t, \quad k \in \{1, \dots, n\},$$

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Considering the empirical distribution $\nu^n = \frac{1}{n} \sum_{k=1}^n \delta_{x_k}$, one has

$$f_n(\theta;x) = \frac{1}{n} \sum_{k=1}^n \Phi(\theta,x_k) = \langle \Phi(\theta,\cdot), \nu^n \rangle.$$

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The expression for $x_k(t)$ looks as an Euler scheme for

$$egin{aligned} dX_k(t) &= V(X_k(t), \mu_t) dt, \ \mu_t &= rac{1}{n} \sum_{k=1}^n \delta_{X_k(t)}, \quad V(x, \mu) = \mathbb{E}_{\theta} V(x, \mu, \theta). \end{aligned}$$

Convergence to deterministic SPDE

If $x_k(0) \sim \mu_0$ – i.i.d. and $\Delta t = \frac{1}{n}$, then

$$d(\nu_t^n, \mu_t) = O\left(\frac{1}{\sqrt{n}}\right),$$

where μ_t solves

$$d\mu_t = -\nabla \left(V(\cdot, \mu_t)\mu_t\right)dt$$

with

$$V(x,\mu) = \mathbb{E}_{\theta} V(x,\mu,\theta) = \nabla F(x) - \langle \nabla_x K(x,\cdot), \mu \rangle$$

and

$$F(x) = \mathbb{E}_{\theta} f(\theta) \Phi(\theta, x), \quad K(x, y) = \mathbb{E}_{\theta} [\Phi(\theta, x) \Phi(\theta, y)].$$

[Mei, Montanari, Nguyen '18]



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 \implies The mean behavior of the SGD dynamics can then be analysed by considering μ_t .

Main Goal

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Goal: Propose an SPDE which would capture the fluctuations of the SGD dynamics and also would give its better approximation.

Stochastic gradient descent

$$x_k(t_{i+1}) = x_k(t_i) + V(x_k(t_i), \nu_{t_i}^n, \theta_i) \Delta t$$

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is the Euler-Maruyama scheme for the SDE

$$dX_k(t) = V(X_k(t), \mu_t^n) dt + \sqrt{\alpha} (\Sigma^{\frac{1}{2}})_k(X(t)) dB(t), \quad k \in \{1, \dots, n\}$$

where $\mu_t^n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i(t)}$, $\Sigma_{k,l}(x) = \mathbb{E}_{\theta} G(x_k, \mu, \theta) \otimes G(x_l, \mu, \theta)$ and B - n-dim Brownian motion.

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 \rightarrow $\Sigma^{\frac{1}{2}}$ is $dn \times dn$ matrix!



SDE Driven by Inf-Dim Noise for SGD Dynamics

Stochastic gradient descent

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[Gess, Kassing, K. '23]

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$$d\mu_t = -\nabla \cdot (V(\cdot, \mu_t)\mu_t)dt$$

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The martingale problem for this equation was considered in [Rotskoff, Vanden-Eijnden, CPAM, '22]

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Well-posedness results for similar SPDEs:

• Continuity equation in the fluid dynamics and optimal transportation [Ambrosio, Trevisan, Crippa...]. There A = G = 0.

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- Particle representations for a class of nonlinear SPDEs [Kurtz, Xiong '99]. The equation has more general form but the initial condition μ_0 must have an L_2 -density w.r.t. the Lebesgue measure.

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The results from [Kurtz, Xiong] can be applied to our equation if μ_0 has L_2 -density!

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Quantified Mean-Field Limit

Well-posedness and superposition principle

Wasserstein Distance

Let (E, d) be a Polish space, and for $p \ge 1$ $\mathcal{P}_p(E)$ be a space of all probability measures ρ on E with

$$\int_{F} d^{p}(x,o)\rho(dx) < \infty.$$

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For $\rho_1, \rho_2 \in \mathcal{P}_p(E)$ we define the **Wasserstein distance** by

$$\mathcal{W}^{p}_{p}(
ho_{1},
ho_{2})=\inf\left\{ \mathbb{E}d^{p}(\xi_{1},\xi_{2}):\ \xi_{i}\sim
ho_{i}
ight\}$$

Higher Order Approximation of SGD

Stochastic Mean-Field Equation:

$$d\mu_t = -\nabla \cdot (V(\cdot, \mu_t)\mu_t)dt + \frac{\alpha}{2}\nabla^2 : (A(\cdot, \mu_t)\mu_t)dt + \sqrt{\alpha}\nabla \cdot \int_{\Theta} G(\cdot, \mu_t, \theta)\mu_t \, W(d\theta, dt)$$
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Theorem 1 (Gess, Gvalani, K. 2022)

- V, G Lipschitz cont. and diff. w.r.t. the special variable with bdd deriv.;
- ν_t^n the empirical process associated to the SGD dynamics with $\alpha = \frac{1}{n}$;
- μ_t^n a (unique) solution to the SMFE started from

$$\mu_0^n = \nu_0^n = \frac{1}{n} \sum_{k=1}^n \delta_{x_k(0)}$$

with $x_k(0) \sim \mu_0$ i.i.d.

Then all $p \in [1,2)$

$$W_p(\text{Law }\mu^n, \text{Law }\nu^n) = o(n^{-1/2}).$$

Quantified Central Limit Theorem for SMFE

Theorem 2 (Gess, Gvalani, K. 2022)

Under the assumptions of the previous theorem, $\eta_t^n := \sqrt{n} \left(\mu_t^n - \mu_t^0 \right) \to \eta_t$ where η_t is a Gaussian process solving

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Moreover,
$$\mathbb{E}\sup_{t\in[0,T]}\|\eta^n_t-\eta_t\|_{-J}^2\leq \frac{C}{n}$$
.

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ight) dt -
abla \cdot \int_{\Theta} G(\cdot,\mu_t^0, heta) \mu_t^0 W(d heta,dt).$$

Moreover, $\mathbb{E} \sup_{t \in [0,T]} \|\eta_t^n - \eta_t\|_{-J}^2 \leq \frac{C}{n}$.

Remark. [Sirignano, Spiliopoulos, '20]

For
$$\tilde{\eta}^n_t := \sqrt{n}(\nu^n_t - \mu^0_t)$$

$$\mathbb{E}\sup_{t \in [0,T]} \|\tilde{\eta}^n_t\|^2_{-J} \leq C \quad \text{and} \quad \tilde{\eta}^n \to \eta.$$

Note that

$$\mu_t^n = \mu_t^0 + n^{-1/2} \eta + O(n^{-1}).$$

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Therefore, $\mu^{n} - \nu^{n} = o(n^{-1/2})$.

$$\begin{split} \sqrt{n^p} \mathcal{W}_p^p \left(\mathsf{Law}(\mu^n), \mathsf{Law}(\nu^n) \right) &= \sqrt{n^p} \inf \mathbb{E} \left[\sup_{t \in [0,T]} \| \mu_t^n - \nu_t^n \|_{-J}^p \right] \\ &= \inf \mathbb{E} \left[\sup_{t \in [0,T]} \| \sqrt{n} (\mu_t^n - \mu_t^0) - \sqrt{n} (\nu_t^n - \mu_t^0) \|_{-J}^p \right] \\ &= \mathcal{W}_p^p \left(\mathsf{Law}(\eta^n), \mathsf{Law}(\tilde{\eta}^n) \right) \to 0. \end{split}$$

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where

$$dX(u,t) = V(X(u,t))dt, \quad X(u,0) = u.$$

[Ambrosio, Trevisan, Lions,...]

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[Ambrosio, Trevisan, Lions,...]

The Stochastic Mean-Field Equation was derived from:

$$dX_k(t) = V(X_k(t), \mu_t^n) dt + \sqrt{\alpha} \int_{\Theta} G(X_k(t), \mu_t^n, \theta) W(d\theta, dt),$$

$$X_k(0) = x_k(0), \quad \mu_t^n = \frac{1}{n} \sum_{i=1}^n \delta_{X_i(t)}.$$

Well-Posedness of SMFE

Theorem 3 (Gess, Gvalani, K. 2022)

Let the coefficients V, G be Lipschitz continuous and smooth enough w.r.t. special variable. Then the SMFE

$$d\mu_t = -\nabla \cdot (V(\cdot, \mu_t)\mu_t) dt + \frac{\alpha}{2} \nabla^2 : (A(\cdot, \mu_t)\mu_t) dt$$

 $-\sqrt{\alpha} \nabla \cdot \int_{\Theta} G(\cdot, \mu_t, \theta)\mu_t W(d\theta, dt)$

has a unique solution. Moreover, μ_t is a superposition solution, i.e.,

$$\mu_t = \mu_0 \circ X^{-1}(\cdot, t), \quad t \ge 0,$$

where X solves

$$dX(u,t) = V(X(u,t), \mu_t)dt + \sqrt{\alpha} \int_{\Theta} G(X(u,t), \mu_t, \theta)W(d\theta, dt)$$
$$X(u,0) = u, \quad u \in \mathbb{R}^d.$$

SDE with Interaction

SDE with interaction:

$$dX(u,t) = V(X(u,t), \mu_t)dt + \sqrt{\alpha} \int_{\Theta} G(X(u,t), \mu_t, \theta)W(d\theta, dt),$$

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Theorem (Kotelenez '95, Dorogovtsev' 07)

Let V, G be Lipschitz continuous, i.e. $\exists L > 0$ such that a.s.

$$|V(x,\mu) - V(y,\nu)| + ||G(x,\mu,\cdot) - G(y,\nu,\cdot)||_{\vartheta} \le L(|x-y| + W_2(\mu,\nu)).$$

Then for every $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$ the SDE with interaction has a unique solution started from μ_0 .

Definition of Solutions to SMFE

$$d\mu_t = -\nabla \cdot (V(\cdot, \mu_t)\mu_t) dt + \frac{\alpha}{2}\nabla^2 : (A(\cdot, \mu_t)\mu_t) dt - \sqrt{\alpha}\nabla \cdot \int_{\Theta} G(\cdot, \mu_t, \theta)\mu_t W(d\theta, dt)$$

Definition of (weak-strong) solution

A continuous (\mathcal{F}_t^W) -adapted process μ_t , $t \geq 0$, in $\mathcal{P}_2(\mathbb{R}^d)$ is a solution to SMFE started from μ_0 if $\forall \varphi \in \mathcal{C}^2_c(\mathbb{R}^d)$ a.s. $\forall t \geq 0$

$$\begin{split} \langle \varphi, \mu_t \rangle &= \langle \varphi, \mu_0 \rangle + \int_0^t \left\langle \nabla \varphi \cdot V(\cdot, \mu_s), \mu_s \right\rangle ds + \frac{\alpha}{2} \int_0^t \left\langle \nabla^2 \varphi : A(\cdot, \mu_s), \mu_s \right\rangle ds \\ &+ \sqrt{\alpha} \int_0^t \int_{\Theta} \left\langle \nabla \varphi \cdot G(\cdot, \mu_s, \theta), \mu_s \right\rangle W(d\theta, ds) \end{split}$$

SMFE and SDE with Interaction

Lemma

Let X be a solution to the SDE with interaction with $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Then $\mu_t = \mu_0 \circ X^{-1}(\cdot, t)$, $t \ge 0$, is a solution to the SMFE.

SMFE and SDE with Interaction

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Definition: We will say that μ_t , $t \ge 0$, is a superposition solution to the Stochastic Mean-Field equation.

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Let X be a solution to the SDE with interaction with $\mu_0 \in \mathcal{P}_2(\mathbb{R}^d)$. Then $\mu_t = \mu_0 \circ X^{-1}(\cdot, t)$, $t \ge 0$, is a solution to the SMFE.

Definition: We will say that μ_t , $t \ge 0$, is a superposition solution to the Stochastic Mean-Field equation.

Corollary

Let V, G be Lipschitz continuous. Then the SMFE

$$egin{aligned} d\mu_t &= -
abla \cdot (V(\cdot,\mu_t)\mu_t) \, dt + rac{lpha}{2}
abla^2 : (A(\cdot,\mu_t)\mu_t) \, dt \ &- \sqrt{lpha}
abla \cdot \int_{\Theta} G(\cdot,\mu_t, heta)\mu_t W(d heta,dt) \end{aligned}$$

has a unique solution iff it has only superposition solutions.

Uniqueness of Solutions to SMFE

• To prove the uniqueness, we show that every solution to the (nonlinear) SMFE is a superposition solution.

Uniqueness of Solutions to SMFE

- To prove the uniqueness, we show that every solution to the (nonlinear) SMFE is a superposition solution.
- We first freeze the solution μ_t in the coefficients, considering the linear SPDE:

$$egin{aligned} d
u_t &= -
abla \cdot \left(
u(t, \cdot)
u_t
ight) dt + rac{lpha}{2}
abla^2 : \left(
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ight) dt \ &- \sqrt{lpha}
abla \cdot \int_{\Theta} g(t, \cdot, heta)
u_t W(d heta, dt), \end{aligned}$$

where $a(t,x) = A(x,\mu_t)$, $v(t,x) = V(x,\mu_t)$ and $g(t,x,\theta) = G(x,\mu_t,\theta)$.

Uniqueness of Solutions to SMFE

- To prove the uniqueness, we show that every solution to the (nonlinear) SMFE is a superposition solution.
- We first freeze the solution μ_t in the coefficients, considering the linear SPDE:

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where
$$a(t,x) = A(x, \mu_t)$$
, $v(t,x) = V(x, \mu_t)$ and $g(t,x,\theta) = G(x, \mu_t,\theta)$.

 We remove the second order term and the noise term from the linear SPDE by a (random) transformation of the space.

Random Transformation of State Space

We introduce the field of martingales

$$M(x,t) = \sqrt{\alpha} \int_0^t g(s,x,\theta) W(d\theta,ds), \quad x \in \mathbb{R}^d, \quad t \geq 0.$$

and consider a solution $\psi_t(x) = (\psi_t^1(x), \dots, \psi_t^d(x))$ to the stochastic transport equation

$$\psi_t^k(x) = x^k - \int_0^t \nabla \psi_s^k(x) \cdot M(x, \circ ds).$$

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Lemma (see Kunita Stochastic flows and SDEs)

Under some smooth assumption on the coefficient g, the exists a field of diffeomorphisms $\psi(t,\cdot):\mathbb{R}^d\to\mathbb{R}^d$, $t\geq 0$, which solves the stochastic transport equation.

Transformed SPDE

For the solution ν_t , $t \geq 0$, to the linear SPDE

$$d
u_t = -
abla \cdot (v(t,\cdot)
u_t) \, dt + rac{lpha}{2}
abla^2 : (a(t,\cdot)
u_t) \, dt - \sqrt{lpha}
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u_t W(d heta,dt),$$

we define

$$\rho_t = \nu_t \circ \psi_t^{-1}.$$

Transformed SPDE

For the solution ν_t , $t \geq 0$, to the linear SPDE

$$d\nu_t = -\nabla \cdot (v(t,\cdot)\nu_t) dt + \frac{\alpha}{2}\nabla^2 : (a(t,\cdot)\nu_t) dt - \sqrt{\alpha}\nabla \cdot \int_{\Theta} g(t,\cdot,\theta)\nu_t W(d\theta,dt),$$

we define

$$\rho_t = \nu_t \circ \psi_t^{-1}.$$

Proposition

Let the coefficient g be smooth enough. Then ρ_t , $t \geq 0$, is a solution to the continuity equation^a

$$d\rho_t = -\nabla (b(t,\cdot)\rho_t)dt, \quad \rho_0 = \nu_0 = \mu_0,$$

for some **b** depending on v and derivatives of a and ψ .

^aAmbrosio, Lions, Trevisan....

$$x_k(0) \sim \mu_0 - \text{i.i.d.}, \ \alpha - \text{learning rate}, \ t_i = i\alpha, \ \theta_i \sim \vartheta - \text{i.i.d.}$$

$$x_k(t_{i+1}) = x_k(t_i) + V(x_k(t_i), \nu_{t_i}^n, \theta_i)\alpha, \quad k \in \{1, \ldots, n\},$$

where $\nu_t^n = \frac{1}{n} \sum_{k=1}^n \delta_{x_k(t)}$.

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where $\nu_t^n = \frac{1}{n} \sum_{k=1}^n \delta_{x_k(t)}$.

$$dX(u,t) = V(X(u,t), \mu_t^n) dt$$

$$+ \sqrt{\alpha} \int_{\Theta} G(X(u,t), \mu_t^n, \theta) W(d\theta, dt),$$

$$X(u,0) = u, \quad \mu_t^n = \nu_0^n \circ X^{-1}(\cdot, t),$$

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$$\Longrightarrow$$
 For $lpha=rac{1}{n}$, $\mathcal{W}_{
ho}(ext{Law}\,\mu^n, ext{Law}\,
u^n)=o(n^{-1/2}).$

 $x_k(0) \sim \mu_0$ – i.i.d., α – learning rate, $t_i = i\alpha$, $\theta_i \sim \vartheta$ – i.i.d.

$$x_k(t_{i+1}) = x_k(t_i) + V(x_k(t_i), \nu_{t_i}^n, \theta_i)\alpha, \quad k \in \{1, \dots, n\},$$

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 For $lpha=rac{1}{n},\;$ +Quantified CLT for SGD $\mathcal{W}_p(ext{Law}\,\mu^n, ext{Law}\,
u^n)=O(n^{-1}).$

 $x_k(0) \sim \mu_0$ – i.i.d., α – learning rate, $t_i = i\alpha$, $\theta_i \sim \vartheta$ – i.i.d.

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$$dX(u,t) = V(X(u,t), \mu_t^n) dt$$

$$+ \sqrt{\alpha} \int_{\Theta} G(X(u,t), \mu_t^n, \theta) W(d\theta, dt),$$

$$X(u,0) = u, \quad \mu_t^n = \nu_0^n \circ X^{-1}(\cdot, t),$$

$$\implies$$
 For $\alpha=\frac{1}{n}$, +Quantified CLT for SGD
$$\mathcal{W}_{p}(\operatorname{Law}\mu^{n},\operatorname{Law}\nu^{n})=O(n^{-1})=O(\alpha).$$

 $x_k(0) \sim \mu_0 - \text{i.i.d.}, \ \alpha - \text{learning rate}, \ t_i = i\alpha, \ \theta_i \sim \vartheta - \text{i.i.d.}$

$$x_k(t_{i+1}) = x_k(t_i) + V(x_k(t_i), \nu_{t_i}^n, \theta_i)\alpha, \quad k \in \{1, \dots, n\},$$

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where W is a cylindrical Wiener process on $L_2(\Theta, P)$.

For
$$U \in \mathcal{C}^4(\mathcal{P}_2)$$

$$\sup_{t \le T} |\mathbb{E} U(\mu_t^n) - \mathbb{E} U(\nu_t^n)| =$$

like in [Li, Tai, E, JMLR, '19] for SGD dynamics.

$$x_k(0) \sim \mu_0 - \text{i.i.d.}, \ \alpha - \text{learning rate}, \ t_i = i\alpha, \ \theta_i \sim \vartheta - \text{i.i.d.}$$

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where W is a cylindrical Wiener process on $L_2(\Theta, P)$.

For
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, and $n \geq 1/\alpha^{4d}$

$$\sup_{t \leq T} |\mathbb{E} U(\mu_t^n) - \mathbb{E} U(\nu_t^n)| = O(\alpha)$$

like in [Li, Tai, E, JMLR, '19] for SGD dynamics.

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where $\nu_t^n = \frac{1}{n} \sum_{k=1}^n \delta_{x_k(t)}$.

$$dX(u,t) = V(X(u,t),\mu_t^n)dt - \frac{\alpha}{4}\nabla|V(X(u,t),\mu_t^n)|^2dt - \frac{\alpha}{4}\langle D|V(X(u,t),\mu_t^n)|^2,\mu_t^n\rangle dt + \sqrt{\alpha}\int_{\Theta}G(X(u,t),\mu_t^n,\theta)W(d\theta,dt),$$

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$$U \in C^4(\mathcal{P}_2)$$
, and $n \geq 1/\alpha^{4d}$

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like in [Li, Tai, E, JMLR, '19] for SGD dynamics.

See [Gess, Kassing, K. '23].

Reference



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Thank you!