Stochastic Modified Flows, Mean-Field Limits and Dynamics of Stochastic Gradient Descent

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Supervised Learning

- Having a large sets of data $\{(\theta_i, \gamma_i),\ i \in I\}$, $\theta_i \sim P$ 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 $x_k \in \mathbb{R}^d$, $k \in \{1, \dots, n\}$, 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**

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

where P is the distribution of θ_i.

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

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Continuous Dynamics of Parameters

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

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

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

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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

$$dX_k(t) = V(X_k(t), \mu_t)dt,$$

$$\mu_t = \frac{1}{n}\sum_{k=1}^n \delta_{X_k(t)}, \quad V(x, \mu) = \mathbb{E}_\theta V(x, \mu, \theta).$$

Convergence to deterministic SPDE

If $x_k(0) \sim \mu_0$ – i.i.d., then

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

where μ_t solves

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

[Mei, Montanari, Nguyen '18]

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Problem. After passing to the deterministic gradient flow μ, all of the information about the inherent fluctuations of the stochastic gradient descent dynamics is lost.

SDE Driven by Inf-Dim Noise for SGD Dynamics

Stochastic gradient descent

$$\begin{aligned} x_k(t_{i+1}) &= x_k(t_i) + V(x_k(t_i), \nu^n_{t_i}, \theta_i)\Delta t \\ &= x_k(t_i) + \underbrace{\mathbb{E}_\theta V(\dots)}_{=V(x_k(t_i),\nu^n_{t_i})}\Delta t + \underbrace{\sqrt{\Delta t}}_{=\sqrt{\alpha}}\underbrace{(V(\dots) - \mathbb{E}_\theta V(\dots))}_{=G(x_k(t_i),\nu^n_{t_i},\theta_i)}\sqrt{\Delta t} \end{aligned}$$

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is the Euler-Maruyama scheme for the SDE

$$dX_k(t) = V(X_k(t), \mu^n_t)dt + \sqrt{\alpha} \int_\Theta G(X_k(t), \mu^n_t, \theta) W(d\theta, dt), \quad k \in \{1, \dots, n\}$$

where $\mu^n_t = \frac{1}{n} \sum_{i=1}^n \delta_{X_i(t)}$, W – white noise on $L_2(\Theta, P)$ (P is the distribution of θ).

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Using Itô 's formula, we come to the **Stochastic Mean-Field Equation:**

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

where $A(x_k, \mu) = \mathbb{E}_\theta G(x_k, \mu) \otimes G(x_k, \mu)$.

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where $A(x_k, \mu) = \mathbb{E}_\theta G(x_k, \mu) \otimes G(x_k, \mu)$.

$\rightsquigarrow$ The martingale problem for this equation is the same as in [Rotskoff, Vanden-Eijnden, CPAM, '22]

Well-Posedness of SMFE

Theorem 1 (Gess, Gvalani, K. 2022)

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

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

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

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

where X solves

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

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Higher Order Approximation of SGD

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Theorem 2 **(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 $p \in [1, 2)$

$$\mathcal{W}_p(\mathrm{Law}\,\mu^n, \mathrm{Law}\,\nu^n) = o(n^{-1/2})$$

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$$\mathcal{W}_p(\mathrm{Law}\,\mu^n, \mathrm{Law}\,\nu^n) = o(n^{-1/2})$$

$$\rightsquigarrow O(n^{-1}), \quad \text{if quintified CLT for SGD holds.}$$

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is the Euler scheme for the SDE

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dX_t = -\nabla R(X_t)dt + \sqrt{\alpha}\Sigma^{\frac{1}{2}}(X_t)dw_t,
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where $\Sigma(x) = \mathbb{E}_P G(x,\theta) \otimes G(x,\theta)$.

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Theorem (Li, Tai, E '19, JMLR)

For f, R and $\Sigma^{\frac{1}{2}}$ smooth enough with bounded derivatives one has

$$\sup_{t_i \le T} |\mathbb{E}f(x_{t_i}) - \mathbb{E}f(X_{t_i})| = O(\alpha).$$

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$$dX_t = -\nabla R(X_t)dt - \frac{\alpha}{4}\nabla|\nabla R(X_t)|^2 dt + \sqrt{\alpha}\Sigma^{\frac{1}{2}}(X_t)dw_t,$$

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Distribution Dependent Stochastic Modified Flow

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

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

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Distribution Dependent Stochastic Flow:

$$\begin{aligned} dX(u,t) &= V(X(u,t), \mu_t)dt \\ &\qquad + \sqrt{\alpha}\int_\Theta G(X(u,t), \mu_t, \theta)W(d\theta, dt), \\ X(u,0) &= u, \quad \mu_t = \mu_0 \circ X_t^{-1}, \end{aligned}$$

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

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Theorem 3 **(Gess, Kassing, K. '24, JMLR)**

Let $\mu_0 \in \mathcal{P}_2$ and V, G be regular enough. Then for every $\Phi \in \mathcal{C}^4_b(\mathcal{P}_2)$

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Distribution Dependent Stochastic Modified Flow

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

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

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$$dX(u,t) = V(X(u,t),\mu_t)dt - \frac{\alpha}{4}\nabla|V(X(u,t),\mu_t)|^2 dt - \frac{\alpha}{4}\langle D|V(X(u,t),\mu_t)|^2, \mu_t\rangle dt$$

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

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Assume that $V(x,\nu,\theta) = -\nabla R(x,\theta)$, then

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Define $X_k(t) := X(x_k(0),t)$, $k \in [n]$. Then for every $f \in \mathcal{C}_b^4(\mathbb{R}^{dn})$

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Stoch. Modified Flow vs Stoch. Modified Equation

Stochastic Modified Flow:

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1. Motivation and derivation of the SPDE

2. Quantified Mean-Field Limit

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4. Idea of Proof

Flow structure of overparameterized SGD

The SGD

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

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$$x(u, t_{i+1}) = x(u, t_i) + V(x(u, t_i), \nu_{t_i}, \theta_i)\Delta t,$$
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by taking $\nu_0 := \nu_0^n$.

Interpolation of One-Step estimate

Set $(t_1 = \Delta t = \alpha)$

$$\mathcal{S}\Psi(\mu_0) := \mathbb{E}_P \Psi(\nu_{t_1}) = \mathbb{E}_P \Psi(\mu_0 \circ x(\cdot, t_1))^{-1})$$

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$$= \sum_{i=0}^{n-1} \left(\mathcal{S}^{n-i} \mathcal{T}_{t_i} \Phi(\mu_0) - \mathcal{S}^{n-i-1} \mathcal{T}_{t_{i+1}} \Phi(\mu_0) \right)$$

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$$= \sum_{i=0}^{n-1}\mathcal{S}^{n-i-1}\left(\mathcal{S}\mathcal{T}_{t_i}\Phi(\mu_0) - \mathcal{T}_\alpha\underbrace{\mathcal{T}_{t_i}\Phi(\mu_0)}_{=:U(t_i,\mu_0)}\right).$$

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$$= \sum_{i=0}^{n-1} \Big(\mathcal{S}^{n-i} \mathcal{T}_{t_i} \Phi(\mu_0) - \mathcal{S}^{n-i-1} \mathcal{T}_{t_{i+1}} \Phi(\mu_0) \Big)$$

$$= \sum_{i=0}^{n-1} \mathcal{S}^{n-i-1} \left(\mathcal{S}\mathcal{T}_{t_i}\Phi(\mu_0) - \mathcal{T}_\alpha \underbrace{\mathcal{T}_{t_i}\Phi(\mu_0)}_{=:U(t_i,\mu_0)} \right).$$

Since $\sup_{\mu_0 \in \mathcal{P}_2} |\mathcal{S}\Psi(\mu_0)| \le \sup_{\mu_0 \in \mathcal{P}_2} |\Psi(\mu_0)|$,

$$\sup_{\mu_0 \in \mathcal{P}} \left| \mathbb{E}\Phi(\mu_0 \circ x(\cdot, t_n)^{-1}) - \mathbb{E}\Phi(\mu_0 \circ X(\cdot, t_n)^{-1}) \right| \le \sum_{i=0}^{n-1} \sup_{\mu_0 \in \mathcal{P}_2} |\mathcal{S}U(t_i, \mu_0) - \mathcal{T}_\alpha U(t_i, \mu_0)|.$$

Expansions of $S\Psi(\mu_0)$ and $P_\alpha\Psi(\mu_0)$

Expansion in Taylor's series w.r.t $\alpha = \Delta t$

$$\mathcal{S}\Psi(\mu_0) = \Psi(\mu_0) + \alpha \int_{\mathbb{R}^d} D\Psi(z,\mu_0) \cdot V(z,\mu_0)\mu_0(dz)$$
$$+ \alpha^2(\dots) + \alpha^3 R_1(\Psi,\mu_0),$$

where $\sup_{\mu_0 \in \mathcal{P}_2} |R_1| \leq C\|\Psi\|_{\mathcal{C}_b^3}$.

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Iterating the equality above, one gets

$$P_\alpha\Psi(\mu_0) = \Psi(\mu_0) + \alpha\mathcal{L}_1\Psi(\mu_0) + \alpha^2\left(\mathcal{L}_2 + \frac{1}{2}\mathcal{L}_1^2\right)\Psi(\mu_0) + \alpha^3 R_2(\Psi,\mu_0),$$

where $\sup_{\mu_0\in\mathcal{P}_2} |R_2| \le C\|\Psi\|_{\mathcal{C}_b^4}$.

Comparison of Generators and End of Proof

For $t_n = \alpha n \leq T$

$$\sup_{\mu_0 \in \mathcal{P}} \left| \mathbb{E}\Phi(\mu_0 \circ Z_{t_n}^{-1}) - \mathbb{E}\Phi(\mu_0 \circ X_{t_n}^{-1}) \right| \leq \sum_{i=0}^{n-1} \sup_{\mu_0 \in \mathcal{P}_2} \left| \mathcal{S}U(t_i, \mu_0) - P_\alpha U(t_i, \mu_0) \right|$$

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$$\leq \sum_{i=0}^{n-1} \sup_{\mu_0 \in \mathcal{P}_2} \alpha^3 \left| R_1(U(t_i, \mu_0), \mu_0) - R_2(U(t_i, \mu_0), \mu_0) \right|$$

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&\leq \alpha^3 n C \|U\|_{\mathcal{C}_b^{0,4}([0,T] \times \mathcal{P}_2)} \leq C_1 T \alpha^2.
\end{aligned}$$

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Proposition **[Feng-Yu Wang, J. Evol. Equ., '21]**

Let $V \in \mathcal{C}_b^{5,5}(\mathbb{R}^d \times \mathcal{P}_2)$, $G(\cdot, \cdot, \theta) \in \mathcal{C}_b^{4,4}(\mathbb{R}^d \times \mathcal{P}_2)$ P-a.s. Then for every $\Phi \in \mathcal{C}_b^4(\mathcal{P}_2)$ the function $U(t, \mu_0) = \mathbb{E}\Phi(\mu_t)$ is a unique solution to the equation

$$\partial_t U(t, \mu_0) = \mathcal{L}_t U(t, \mu_0),$$
$$U(0, \mu_0) = \Phi(\mu_0).$$

Moreover, $U \in \mathcal{C}_b^{0,4}([0, T] \times \mathcal{P}_2)$ and $\partial_t U \in \mathcal{C}([0, T] \times \mathcal{P}_2)$.

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Thank you!