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

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joint work with Benjamin Gess, Rishabh Gvalani and Sebastian Kassing

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Stochastic Gradient Descent:

taking $z(0) \in \mathbb{R}^d$ define

$$z(t_{i+1}) = z(t_i) - \alpha \nabla_z R(z(t_{i+1}), \xi_i)$$

for learning rate α, $t_i = \alpha i$ and $\xi_i \sim P$ – i.i.d.

SGD and ODE

For $\alpha \to 0$ the SDG dynamics

$$z(t_{i+1}) = z(t_i) - \alpha \nabla_z R(z(t_{i+1}), \xi_i)$$

behaves as a solution to ODE

$$dZ_t = -\nabla_z R(Z_t)dt,$$

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Theorem [see e.g. in Li, Tai, E '19, JMLR]

For f and R smooth enough one has

$$\sup_{t_i \leq T} |\mathbb{E} f(z(t_i)) - \mathbb{E} f(Z_{t_i})| = O(\alpha).$$

SGD and SDE

The ODE loses all information about the randomness in the SGD.

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z(t_{i+1}) &= z(t_i) - \alpha \nabla R(z(t_i), \xi_i) \\
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is the Euler scheme for the SDE

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

where $\Sigma(z) = \mathrm{Cov}\left(\nabla R(z, \xi), \nabla R(z, \xi)\right) = \mathbb{E}_P G(z, \xi) \otimes G(z, \xi)$.

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Limitations of Modified SDE

Limited regularity of $\Sigma^{\frac{1}{2}}$:

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Let $z_k(t_i)$ be the SGD dynamics started from $z_k(0)$

$$z_1(t_{i+1}) = z_1(t_i) - \alpha \nabla R(z_1(t_i), \xi_i)$$

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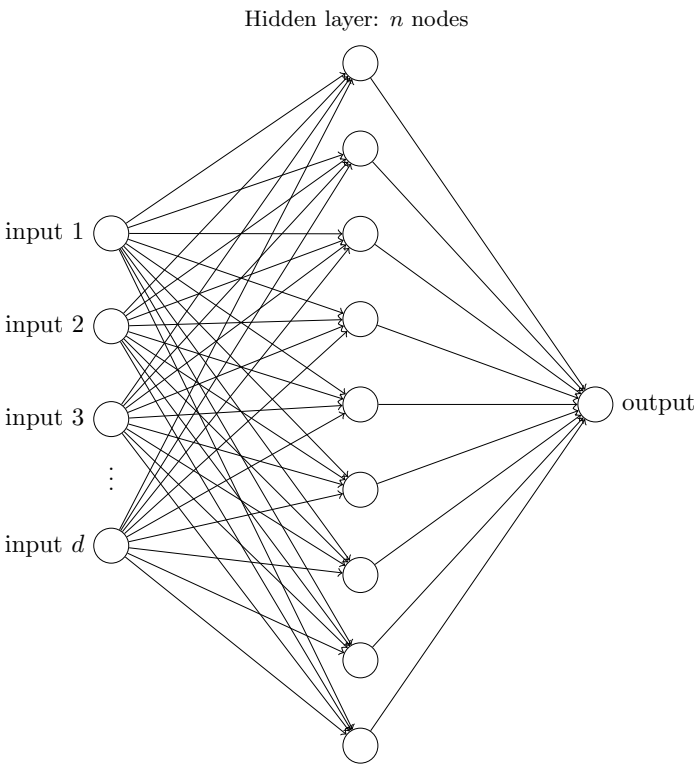
Then

$$(z_1(t_i), \dots, z_n(t_i)) \not\approx (Z^1_{t_i}, \dots, Z^n_{t_i}).$$

for solutions of the (Modified) SDE started from $Z^k_0 = z_k(0)$ since, formally,

$$\mathrm{Cov}\left(z_k, z_l\right) = \mathrm{Cov}\left(\nabla R(z_k, \xi), \nabla R(z_l, \xi)\right) \neq \Sigma^{\frac{1}{2}}\left(Z^k\right)\Sigma^{\frac{1}{2}}\left(Z^l\right) = \mathrm{Cov}\left(Z^k, Z^l\right)$$

Neural Network with One Hidden Layer



Network with a single hidden layer:

$$f_z(\xi) = \frac{1}{n}\sum_{k=1}^{n} \Phi_{z_k}(\xi)$$

$$= \int \Phi_z(\xi)\mu^n(dz) = \langle \Phi(\xi), \mu^n \rangle ,$$

where $z_k \in \mathbb{R}^d$, $k = 1, \ldots, n$, are parameters which have to be found and

$$\mu^n = \frac{1}{n}\sum_{k=1}^{n} \delta_{z_k}$$

[Chizat, Bach, Mei, Nguye, Rotskoff, Sirignano, Vanden-Eijnden...]

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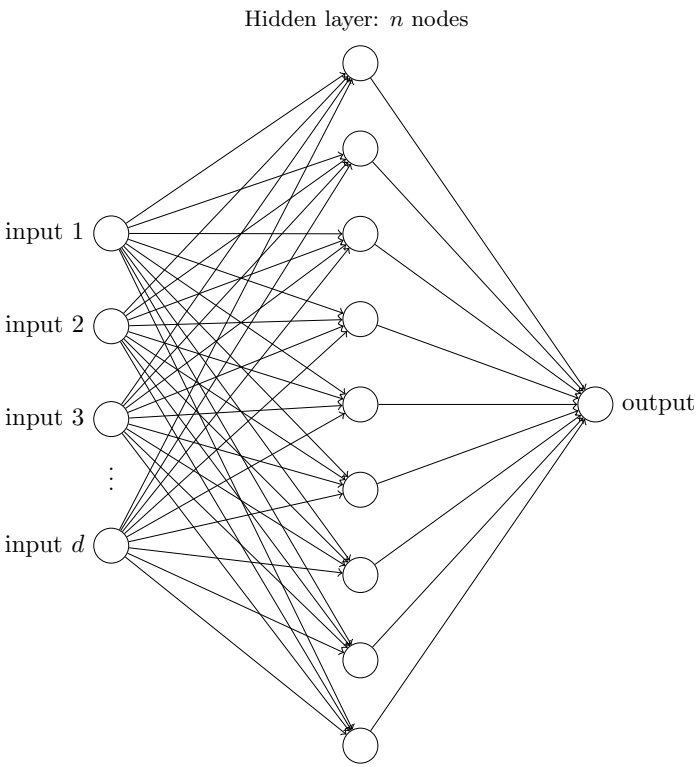

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Risk Function: for $\mathbf{z} = (z_1, \ldots, z_n)$

$$\tilde{R}(\mathbf{z}) := \frac{1}{2}\mathbb{E}_P\left[\left(f(\xi) - f_{\mathbf{z}}(\xi)\right)|^2\right] =: \mathbb{E}\left[\tilde{R}(z_1, \ldots, z_n, \xi)\right] \to \min$$

SGD for Shallow Network

Taking $z_k(0) \sim \mu_0$ i.i.d. and $\xi_i \sim P$ i.i.d. we consider the SGD

$$\mathbf{z}(t_{i+1}) = \mathbf{z}(t_i) - \alpha \nabla_{\mathbf{z}} \tilde{R}\left(\mathbf{z}(t_i), \xi_i\right).$$

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A simple computation shows

$$\begin{aligned} z_1(t_{i+1}) &= z_1(t_i) - \alpha \nabla_{z_1} R\left(z_1(t_i), \mu^n_{t_i}, \xi_i\right) \\ &\dots \\ z_n(t_{i+1}) &= z_n(t_i) - \alpha \nabla_{z_n} R\left(z_n(t_i), \mu^n_{t_i}, \xi_i\right) \end{aligned}$$

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The coefficients depend on n!

Mean-Field ODE (Continuity Equation)

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can be captured for $\alpha \to 0$ by

$$dZ^k_t = -\nabla_{Z^k} R\left(Z^k_t, \nu^n_t\right) dt,$$

with $\nu^n_t = \frac{1}{n}\sum_{k=1}^n \delta_{Z^k_t}$ and $R(z, \nu) = \mathbb{E}\left[R(z, \nu, \xi)\right]$.

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One can write the equation for ν^n_t

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Then $Z^k_t = Z_t(z_k(0))$ and $\nu^n_t = \nu_t$.

Martingale Problem for Empirical distribution

Recall

$$d\mathbf{Z}_t = -\nabla \tilde{R}(\mathbf{Z}_t)dt + \sqrt{\alpha}\Sigma^{\frac{1}{2}}(\mathbf{Z}_t)dw_t$$

captures the motion of

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Taking $\varphi \in C^2_c(\mathbb{R}^d)$, we get for the empirical measure $\nu^n_t = \frac{1}{n}\sum_{k=1}^n \delta_{Z^k_t}$

$$\langle \varphi, \nu^n_t \rangle = \langle \varphi, \nu^n_0 \rangle - \int_0^t \langle \nabla\varphi \cdot \nabla R(\cdot, \nu^n_s), \nu^n_s \rangle \, ds + \frac{\alpha}{2}\int_0^t \left\langle \nabla^2\varphi : A(\cdot, \nu^n_s), \nu^n_s \right\rangle ds + \text{Mart.},$$

with

$$\frac{d}{dt}\left[\text{Mart.}\right]_t = \alpha \int\int (\nabla\varphi(x) \otimes \nabla\varphi(y)) : \tilde{A}(x, y, \nu^n_t)\nu^n_t(dx)\nu^n_t(dy)$$

where $\tilde{A}(z, y, \mu) = \mathrm{Cov}\left(\nabla R(z, \mu, \xi), \nabla R(z, \mu, \xi)\right)$ and $A(z, \mu) = A(z, z, \mu)$

[Rotskoff, Vanden-Eijnden, CPAM, 2022]

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$\rightsquigarrow$ Complicated to work

SDE with Inf-Dim Noise

We repeat the derivation of the equation for SGD with new idea:

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Note that $\mathrm{Cov}\,(z_k, z_l) = \mathbb{E}\,[G(z_k, \mu, \xi) \otimes G(z_l, \mu, \xi)]$

We get

$$dZ^k_t = -\nabla R(Z^k_t, \nu^n_t)dt + \sqrt{\alpha} \underbrace{\int_\Xi G(Z^k_t, \nu^n_t, \xi) W(d\xi, dt)}_{=\sum_l (G, e_l)_{L_2} dw_l(t)}, \quad k = 1, \dots, n,$$

where $\mu^n_t = \frac{1}{n}\sum_{i=1}^n \delta_{Z^k}$, and $W(\xi, t) = \sum_l e_l(\xi) w_l(t)$ is white noise on $L_2(\Xi, P)$

($P = \mathrm{Law}\xi$, Ξ is the state space for ξ) .

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

Connection with SGD

Recall that $z_k(0) \sim \mu_0$ – i.i.d., α – learning rate, $t_i = \alpha i$, $\xi_i \sim P$ – i.i.d.

$$z_k(t_{i+1}) = z_k(t_i) - \alpha \nabla R(z_k(t_i), \mu^n_{t_i}, \xi_i), \quad k = 1, \dots, n$$

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Theorem [Gess, Kassing, K. '24, JMLR]

Let $\mu_0 \in \mathcal{P}_2$ and $\nabla R(z, \nu, \xi)$ be regular enough in z, ν. Then for every $\Phi \in \mathrm{C}^4_b(\mathcal{P}_2)$

$$\sup_{t_i \le T} |\mathbb{E}\Phi(\nu_{t_i}) - \mathbb{E}\Phi(\mu^n_{t_i})| \le C\alpha red^2 + C\sqrt{\mathbb{E}W_2^2(\mu_0, \mu^n_0)}.$$

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n-point motion for SGD

Recall SGD:

$$z_k(t_{i+1}) = z_k(t_i) - \alpha \nabla R(z_k(t_i), \xi_i), \quad k = 1, \dots, n,$$

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Theorem [Gess, Kassing, K. '24, JMLR]

Define $Z_t^k := Z_t(x_k(0))$, $k = 1, \dots, n$. Then for every $f \in C_b^4(\mathbb{R}^{dn})$

$$\sup_{t_i \le T} \left| \mathbb{E} f\left(z_1(t_i), \dots, z_n(t_i)\right) - \mathbb{E} f\left(Z_{t_i}^1, \dots, Z_{t_i}^n\right) \right| \le C\alpha^2.$$

Weak Topology vs. Strong Topology

Observe that for a 1-d Brownian motion w the error between $\sqrt{\alpha}w_t$ and 0 can is different in different topologies

$$W_1\left(\mathrm{Law}\left(\sqrt{\alpha}w_t\right), \delta_0\right) = \mathbb{E}\left[\left|\sqrt{\alpha}w_t - 0\right|\right] = O\left(\sqrt{\alpha}\right)$$

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but

$$\mathbb{E}\left[f\left(\sqrt{\alpha}w_t\right)\right] - \mathbb{E}\left[f(0)\right] = \mathbb{E}\left[f'(0)\sqrt{\alpha}w_t + \frac{1}{2}f''(\theta)\alpha w_t^2\right] = O\left(\|f''\|\alpha\right)$$

Comparison in Wasserstein (strong) topology

SDE for overparametrized shallow neural network with $z_k(0) \sim \mu_0$ i.i.d.

$$z_k(t_{i+1}) = z_k(t_i) - \alpha \nabla_{z_k} R\left(z_k(t_i), \mu^n_{t_i}, \xi_i\right), \quad k = 1, \dots, n.$$

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Theorem [Mei, Montanari, Nguyen '18, PNAS]

For R quite regular smooth enough and $n \sim \frac{1}{\alpha}$ one has

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Proof is based on CLT for SGD [Sirignano, Spiliopoulos '19, SPA] + CLT for the SPDE

References

[1] Gess, Kassing, Konarovskyi,
Stochastic Modified Flows, Mean-Field Limits and Dynamics of Stochastic Gradient Descent
Journal of Machine Learning Research 25 (2024)

[2] Gess, Gvalani, Konarovskyi,
Conservative SPDEs as Fluctuating Mean Field Limits of Stochastic Gradient Descent
Probability Theory and Related Fields 192 (2025)

Thank you!