Stochastic Approximations, Diffusion Limit and Small Random Perturbations of Dynamical Systems

– a probabilistic approach to machine learning.

Wenqing Hu. ¹

¹ Department of Mathematics and Statistics, Missouri S&T.
Deep Neural Network (DNN). Goal is to solve the following stochastic optimization problem

$$\min_{x \in \mathbb{R}^d} F(x) \equiv \frac{1}{M} \sum_{i=1}^{M} F_i(x)$$

where each component $F_i$ corresponds to the loss function for data point $i \in \{1, ..., M\}$, and $x$ is the vector of weights being optimized.
Machine Learning Background: Training DNN via minibatch Stochastic Gradient Descent (SGD).

- Naive Thinking: Gradient Descent (GD) updates as

  \[ x^{(t)} = x^{(t-1)} - \eta \left( \frac{1}{M} \sum_{i=1}^{M} \nabla F_i(x^{(t-1)}) \right). \]

- Learning rate \( \eta > 0 \) is usually a small stepsize.
- Access of all gradients \( \nabla F_i(x^{(t-1)}) \) for \( i = 1, \ldots, M \) is in general very expensive in large-scale machine learning problems.
Let $B$ be the minibatch of prescribed size uniformly sampled from $\{1, \ldots, M\}$, then the objective function can be further written as the expectation of a stochastic function

$$
\frac{1}{M} \sum_{i=1}^{M} F_i(x) = \mathbb{E}_B \left( \frac{1}{|B|} \sum_{i \in B} F_i(x) \right) \equiv \mathbb{E}_B F(x; B).
$$

SGD updates as

$$
x(t) = x(t-1) - \eta \left( \frac{1}{|B_t|} \sum_{i \in B_t} \nabla F_i(x(t-1)) \right),
$$

which is the classical mini–batch version of the SGD.
Stochastic Optimization.

- Stochastic Optimization Problem

\[
\min_{x \in U \subset \mathbb{R}^d} F(x).
\]

\[
F(x) \equiv \mathbb{E}[F(x; \zeta)].
\]

- Index random variable $\zeta$ follows some prescribed distribution $\mathcal{D}$. 


We target at finding a local minimum point $x^*$ of the expectation function $F(x) \equiv \mathbb{E}[F(x; \zeta)]$:

$$x^* = \arg \min_{x \in U \subset \mathbb{R}^d} \mathbb{E}[F(x; \zeta)].$$

- Stochastic Gradient Descent (SGD) has iteration:

\[ x^{(t)} = x^{(t-1)} - \eta \nabla F(x^{(t-1)}; \zeta_t), \]

where \( \{\zeta_t\} \) are i.i.d. random variables that have the same distribution as \( \zeta \sim \mathcal{D} \).
Closer look at SGD.

- **SGD:**
  \[ x^{(t)} = x^{(t-1)} - \eta \nabla F(x^{(t-1)}; \zeta_t) \, . \]

- **\( F(x) \equiv \mathbb{E} F(x; \zeta) \)** in which \( \zeta \sim \mathcal{D} \).

- Let
  \[ e_t = \nabla F(x^{(t-1)}; \zeta_t) - \nabla F(x^{(t-1)}) \]

and we can rewrite the SGD as
  \[ x^{(t)} = x^{(t-1)} - \eta (\nabla F(x^{(t-1)}) + e_t) \, . \]
Diffusion Limit of SGD.

- Stochastic difference equation:

\[ x(t) - x(t-1) = -\eta \nabla F(x^{(t-1)}) - \eta e_t . \]

- When \( \eta \) is small, we can approximate \( x(t) \) by a diffusion process \( X_t \) driven by the stochastic differential equation

\[
dX_t = -\eta \nabla F(X_t) dt + \eta \sigma(X_t) dW_t , \quad X_0 = x^{(0)} ,
\]

where \( W_t \) is a standard Brownian motion in \( \mathbb{R}^d \) and

\[ \sigma(x)\sigma^T(x) = D(x) . \]

- The diffusion matrix (noise covariance matrix)

\[ D(x) = E(\nabla F(x; \zeta) - \nabla F(x))(\nabla F(x; \zeta) - \nabla F(x))^T . \]
Diffusion Limit of SGD: Justification.

- **Slogan**: Continuous Markov processes are characterized by its local statistical characteristics only in the first and second moments (conditional mean and (co)variance).
- Such an approximation has been justified in the weak sense in many classical literature. It can also be thought of as a normal deviation result (Hu–Li–Li–Liu, 2018).
- Conversely, the discrete iteration can be viewed as a numerical scheme for the diffusion limit $X_t$.
- In many CS literature people simply refer to the diffusion limit as the SGD algorithm.
Small random perturbations of dynamical systems: gradient flow case.

- **Diffusion Limit of SGD:**
  
  \[ dX_t = -\eta \nabla F(X_t)dt + \eta \sigma(X_t)dW_t, \quad X_0 = x^{(0)} . \]

- Let \( Y_t = X_t/\eta \), then
  
  \[ dY_t = -\nabla F(Y_t)dt + \sqrt{\eta} \sigma(Y_t)dW_t, \quad Y_0 = x^{(0)} . \]

(Random perturbations of the gradient flow!)

- In many CS literature people simply refer to the randomly perturbed process \( Y_t \) as the SGD algorithm.
Summary: Probabilistic Approach.

- Stochastic approximation
  - Small learning rate
  - Diffusion limit

- Training algorithm
  - Statistical properties of learning model (convergence, generalization, ...)
  - Small random perturbations of dynamical systems
SGD as a randomly perturbed gradient flow.

- SGD as a randomly perturbed gradient flow:

\[
\begin{align*}
  dY_t &= -\nabla F(Y_t) dt + \sqrt{\eta} \sigma(Y_t) dW_t , \ Y_0 = x^{(0)} .
\end{align*}
\]

- \( \sigma(x)\sigma^T(x) = D(x) . \)

- The diffusion matrix (noise covariance matrix)

\[
D(x) = E(\nabla F(x; \zeta) - \nabla F(x))(\nabla F(x; \zeta) - \nabla F(x))^T .
\]
Target Problem 1: Convergence Time.

- Assume isotropic noise $D(x) = I_d$.
- Diffusion Limit:
  
  $$dX_t = -\eta \nabla F(X_t)dt + \eta dW_t, \quad X_0 = x^{(0)}.$$  

- Convergence Time = Hitting time
  
  $$\tau^\eta = \inf\{t \geq 0 : F(X_t) \leq F(x^*) + e\}$$  

  for some small $e > 0$.

- Asymptotic of $E\tau^\eta$ as $\eta \to 0$?
Target Problem 1: Convergence Time.

- **Random perturbations**: Let \( Y_t = X_{t/\eta} \), then
  \[
  dY_t = -\nabla F(Y_t) dt + \sqrt{\eta} dW_t, \quad Y_0 = x^{(0)}.
  \]

- **Hitting time**
  \[
  T^\eta = \inf\{ t \geq 0 : F(Y_t) \leq F(x^*) + e \}
  \]
  for some small \( e > 0 \).

- \( \tau^\eta = \eta^{-1} T^\eta \).

- Asymptotic of \( E T^\eta \) as \( \eta \to 0 \)?
Approach to Target Problem 1: Where is the difficulty?

**Figure 1** – Various critical points and the landscape of $F$. 
Approach to Target Problem 1: Where is the difficulty?

- Algorithm spends most of its time near critical points of loss function $F$. 
Approach to Target Problem 1: Escape from a saddle point.

Figure 2 – Escape from a saddle point.
Approach to Target Problem 1: Chain of saddle points.

Figure 3 – Chain of saddle points.
Approach to Target Problem 1: Sequence of stopping times.

- Standard Markov cycle type argument.
- But the geometry is a little different from the classical arguments for elliptic equilibriums found in Freidlin–Wentzell book.
- \( E T^\eta \lesssim \frac{k}{2\gamma_1} \ln(\eta^{-1}) \) conditioned upon convergence.
Approach to Target Problem 1: Convergence Time.

Theorem (Hu-Li, 2017) (i) For any small $\rho > 0$, with probability at least $1 - \rho$, the diffusion limit $X_t$ of SGD converges to the minimizer $x^*$ for sufficiently small $\eta$ after passing through all $k$ saddle points $O_1, \ldots, O_k$.

(ii) Consider the stopping time $\tau_\eta$. Then as $\eta \downarrow 0$, conditioned on the above convergence of the diffusion limit $X_t$ of SGD, we have

$$\lim_{\eta \to 0} \frac{E\tau_\eta}{\eta^{-1} \ln \eta^{-1}} \leq \frac{k}{2\gamma_1}.$$
Target Problem 2: Effect of batchsize on generalization.

- It is believed that escape from “bad minima” to “good minima” is responsible for good empirical properties under SGD training, e.g. generalization.
- DNN training: How batchsize affect the escape properties from local minimum points?
- Large batch training v.s. small batch training.
- Large–batch methods tend to converge to sharp minimizers of the training and testing functions.
- Small–batch methods consistently converge to flat minimizers.

\[
\begin{align*}
\text{Sharp minima} & \rightarrow \text{Poorer generalization} \\
\text{Flat minima} & \rightarrow \text{Better generalization}
\end{align*}
\]
Machine Learning Background: Training DNN via minibatch Stochastic Gradient Descent (SGD).

- Let $B$ be the minibatch of prescribed size uniformly sampled from $\{1, \ldots, M\}$, then the objective function can be further written as the expectation of a stochastic function

$$
\frac{1}{M} \sum_{i=1}^{M} F_i(x) = \mathbb{E}_B \left( \frac{1}{|B|} \sum_{i \in B} F_i(x) \right) \equiv \mathbb{E}_B F(x; B).
$$

- SGD updates as

$$
x(t) = x(t-1) - \eta \left( \frac{1}{|B_t|} \sum_{i \in B_t} \nabla F_i(x(t-1)) \right),
$$

which is the classical mini–batch version of the SGD.
Approach to Target Problem 2: Relationship between batchsize and the diffusion matrix $D(x)$.

- Relationship between batchsize and the diffusion matrix $D(x)$ (Hu-Li-Li-Liu, 2018).

\[
D(x) = \left( \frac{1}{|B|} - \frac{1}{M} \right) D_0(x),
\]

where

\[
D_0(x) = \frac{1}{M - 1} \sum_{i=1}^{M} (\nabla F_i(x) - \nabla F(x)) (\nabla F_i(x) - \nabla F(x))^T.
\]

- Naively, the larger $D(x)$ is, the easier to escape due to injection of the noise.
SGD as a randomly perturbed gradient flow.

- SGD as a randomly perturbed gradient flow:
  \[ dY_t = -\nabla F(Y_t) dt + \sqrt{\eta} \sigma(Y_t) dW_t, \quad Y_0 = x^{(0)}. \]

- The diffusion matrix (noise covariance matrix)
  \[ \sigma(x)\sigma^T(x) = D(x). \]

- The diffusion matrix (noise covariance matrix)
  \[ D(x) = \mathbf{E}(\nabla F(x; \zeta) - \nabla F(x))(\nabla F(x; \zeta) - \nabla F(x))^T. \]
Approach to Target Problem 2 : Escape from basin of attractors via Large Deviations Theory.

- **Theorem**

  (Hu-Li-Li-Liu, 2018) Let $U$ be a basin of attractor such that $O \subset U$ is the only minimum of $F(x)$ and assume that the boundary $\partial U$ of the domain $U$ is smooth so that $\nabla F(x), x \in \partial U$ points to the interior of the boundary of $U$, then for $x_0 \in U$ we have the following two asymptotic

  \[ P(x_0, \partial U) \approx \exp \left( -\frac{1}{\eta} \min_{x \in \partial U} \phi_{loc}^{QP}(x; O) \right), \]

  and

  \[ E_\tau(x_0, \partial U) \approx \frac{1}{\eta} \exp \left( \frac{1}{\eta} \min_{x \in \partial U} \phi_{loc}^{QP}(x; O) \right). \]
Approach to Target Problem 2: The quasi–potential.

- **The local quasi–potential**

\[ \phi_{\text{loc}}^{\text{QP}}(x; x_0) = \inf_{T > 0} \inf_{\psi(0) = x_0, \psi(T) = x} S_{0T}(\psi). \]

- **Action functional** (Large Deviations Rate Function):

\[ S_{0T}(\psi) = \begin{cases} 
\frac{1}{2} \int_0^T \left( \psi_t + \nabla F(\psi_t) \right)^T D^{-1}(\psi_t) \left( \psi_t + \nabla F(\psi_t) \right) dt, & \text{if } \psi_t \text{ is abs. cont. } t \in [0, T]; \\
+\infty, & \text{otherwise}. 
\end{cases} \]
Target Problem 3: Algorithm’s implicit selection of specific local minima.

- Implicit Regularization: It is widely believed that SGD is an implicit regularizer which helps itself to search for a local minimum that is easy to generalize.
- How to understand this phenomenon?
Approach to Target Problem 3: Structure of diffusion matrix $D(x)$.

- Covariance structure (diffusion matrix) $D(x)$ depends implicitly on the model architecture:

  \[ D(x) = \mathbf{E}(\nabla F(x; \zeta) - \nabla F(x))(\nabla F(x; \zeta) - \nabla F(x))^T. \]

- Anisotropic Noise v.s. Isotropic Noise.
- $D(x)$ may have very large condition number!
SGD as a randomly perturbed gradient flow.

- SGD as a randomly perturbed gradient flow:
  \[
  dY_t = -\nabla F(Y_t)dt + \sqrt{\eta} \sigma(Y_t)dW_t , \quad Y_0 = x^{(0)}. 
  \]

- The diffusion matrix (noise covariance matrix)
  \[
  \sigma(x)\sigma^T(x) = D(x). 
  \]
Approach to Target Problem 2: Escape from basin of attractors via Large Deviations Theory.

Theorem (Hu-Li-Li-Liu, 2018) Let $U$ be a basin of attractor such that $O \subset U$ is the only minimum of $F(x)$ and assume that the boundary $\partial U$ of the domain $U$ is smooth so that $\nabla F(x), x \in \partial U$ points to the interior of the boundary of $U$, then for $x_0 \in U$ we have the following two asymptotic

\[
P(x_0, \partial U) \asymp \exp \left( -\frac{1}{\eta} \min_{x \in \partial U} \phi_{QP}^{loc}(x; O) \right),
\]

and

\[
E_T(x_0, \partial U) \asymp \frac{1}{\eta} \exp \left( \frac{1}{\eta} \min_{x \in \partial U} \phi_{QP}^{loc}(x; O) \right).
\]
Approach to Target Problem 2: The quasi–potential.

▶ The local quasi–potential

\[ \phi_{\text{loc}}^{QP}(x; x_0) = \inf_{T > 0} \inf_{\psi(0) = x_0, \psi(T) = x} S_{0T}(\psi). \]

▶ Action functional (Large Deviations Rate Function):

\[
S_{0T}(\psi) = \begin{cases} 
\frac{1}{2} \int_0^T (\psi_t + \nabla F(\psi_t))^T D^{-1}(\psi_t)(\psi_t + \nabla F(\psi_t)) \, dt, & \text{if } \psi_t \text{ is abs. cont. } t \in [0, T]; \\
+\infty, & \text{otherwise}.
\end{cases}
\]
Approach to Target Problem 3: Relation between the quasi–potential and the diffusion matrix $D(x)$. 

▶ Theorem  
(Hu-Zhu-Xiong-Huan, 2019) The local quasi–potential $\phi_{loc}^{QP}(x; x_0)$ is a solution to the Hamilton–Jacobi equation

$$\frac{1}{2} \left( \nabla \phi_{loc}^{QP}(x; x_0) \right)^T D(x) \nabla \phi_{loc}^{QP}(x; x_0) - \nabla F(x) \cdot \nabla \phi_{loc}^{QP}(x; x_0) = 0,$$

with boundary condition

$$\phi_{loc}^{QP}(O; x_0) = 0.$$
Approach to Target Problem 3: Escape from local minimum point: Isotropic Noise v.s. Anisotropic Noise.

**Figure 4** – Escape from local minimum point: Isotropic Noise v.s. Anisotropic Noise.
Target Problem 3: Algorithm’s implicit selection of specific local minima.

- Suppose that $F(x)$ is non-convex and admits several local minimum points.
- Does SGD always select the global minimum of $F(x)$?
SGD as a randomly perturbed gradient flow.

- SGD as a randomly perturbed gradient flow:
  
  $$dY_t = -\nabla F(Y_t)dt + \sqrt{\eta}\sigma(Y_t)dW_t, \quad Y_0 = x^{(0)}.$$  

- The diffusion matrix (noise covariance matrix)
  
  $$\sigma(x)\sigma^T(x) = D(x).$$  

- The diffusion matrix (noise covariance matrix)
  
  $$D(x) = \mathbf{E}(\nabla F(x; \zeta) - \nabla F(x))(\nabla F(x; \zeta) - \nabla F(x))^T.$$
Approach to Target Problem 3: Variational Inference.

- **Variational Inference**: Invariant density

\[
\rho^{\text{SS}}(x) = \frac{1}{Z(\eta)} \exp \left( -\frac{2}{\eta} \Phi(x) \right).
\]

- SGD selects the global minimum of \( \Phi(x) \): \( \rho(x, t) \to \rho^{\text{SS}}(x) \) as \( t \to \infty \).

- If diffusion matrix \( D(x) = I_d \) is isotropic, then \( \Phi(x) \propto F(x) \).

- Anisotropic noise is common!

- So in general \( \Phi(x) \neq F(x) \).
Approach to Target Problem 3: Variational Inference via Large Deviation Theory.

- Large Deviation Theory provides another way to express the invariant density

\[ \rho^{SS}(x) \asymp \exp \left( -\frac{1}{\eta} \phi^{QP}(x) \right). \]

- (global) quasi–potential: \( \phi^{QP}(x) \).
Approach to Target Problem 3: Variational Inference via Large Deviation Theory.

- Theorem

  (Hu-Zhu-Xiong-Huan, 2019) SGD selects the global minimum $x^*$ of $\phi^{QP}(x)$ such that $\phi^{QP}(x^*) = 0$. 
The (global) quasi-potential $\phi^{QP}(x)$ can be calculated from the local quasi-potential $\phi_{loc}^{QP}(x; x_0)$.

We have seen that the local quasi-potential $\phi_{loc}^{QP}(x; x_0)$ depends on the diffusion matrix $D(x)$ via the Hamilton-Jacobi equation.

Markov chain on local minimum points (Freidlin–Wentzell theory).
Approach to Target Problem 3: Implicit regularization via covariance structure.

**Figure 5** – Implicit regularization via covariance structure. The loss function is symmetric with respect to two local minima \((-2, 0)\) and \((2, 0)\). Left: Process starts from \((-2, 0)\), anisotropic noise in the potential well; Right: Process starts from \((2, 0)\), isotropic noise in the potential well. SGD tends to select \((2, 0)\).
Summary: Probabilistic Approach.

- Stochastic approximation
  - Small learning rate
  - Diffusion limit

- Training algorithm
  - Statistical properties of learning model (convergence, generalization, ...)
  - Small random perturbations of dynamical systems
Stochastic Approximation: Stochastic heavy–ball method.

\[
\min_{x \in \mathbb{R}^d} f(x) .
\]

“heavy ball method” (B.Polyak 1964)

\[
\begin{aligned}
x_t &= x_{t-1} + \sqrt{s}v_t , \\
v_t &= (1 - \alpha \sqrt{s})v_{t-1} - \sqrt{s} \nabla X f (x_{t-1}) , \\
x_0, v_0 &\in \mathbb{R}^d .
\end{aligned}
\]

Stochastic heavy ball method:

\[
\begin{aligned}
x_t &= x_{t-1} + \sqrt{s}v_t , \\
v_t &= (1 - \alpha \sqrt{s})v_{t-1} - \sqrt{s} \nabla X f (x_{t-1}; \zeta_t) , \\
x_0, v_0 &\in \mathbb{R}^d .
\end{aligned}
\]
Diffusion Limit of Stochastic heavy–ball method.

Diffusion limit of the stochastic heavy ball method:

\[
\begin{aligned}
    dx(t) &= \sqrt{s}v(t)dt , \\
    dv(t) &= -\sqrt{s}\alpha v(t)dt - \sqrt{s}\nabla X f(x(t)) + \sqrt{s}\sigma(x(t))dW_t , \\
    x(0), v(0) &\in \mathbb{R}^d .
\end{aligned}
\]
Small random perturbations of dynamical systems: dissipative Hamiltonian system.

Small random perturbations of dissipated Hamiltonian system:

\[ \begin{align*}
    dX_t^\varepsilon &= V_t^\varepsilon dt; \\
    dV_t^\varepsilon &= (-\alpha V_t^\varepsilon - \nabla \chi f(X_t^\varepsilon))dt + \varepsilon \sigma(X_t^\varepsilon) dW_t, \\
    X_0^\varepsilon, V_0^\varepsilon &\in \mathbb{R}^d.
\end{align*} \]

Hu-Li-Su, 2017 and work in progress.
Many further interesting directions at the interplay of probability and data science ...

- Escape from saddle points for anisotropic noise.
- Can the program on Hamilton–Jacobi equation be carried to specific deep neural network structures?
- Many more applied problems in collaborations with CS/ECE/ORIE people...
Thank you for your attention!